



NMR *SUITE* **3.5**

for Windows XP

Installation Guide

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Chapter 1

Introduction

1.1 About this manual

This manual is the NMR-SUITE 3.5 Installation guide for Windows XP. It is available:

- as pdf file on the NMR-SUITE CDROM
- as XWIN-NMR Online Help: click **Help** → **Installation Guide**
- as the at the time actual version on the Bruker web-server:
`http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html`
- Note that this manual does not contain the NMR-SUITE Release letter. That is a separate document which is not available as a hard copy but delivered as pdf and text files on the NMR-SUITE CDROM and also on the Bruker web-server (you can find it at the same URL as the Installation Guide)

`http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html`

This manual is subdivided into an introduction and three main parts. It depends on your local demands which of these are necessary for you at the moment.

The first part describes the scratch installation of Windows XP and some configu-

ration steps for Windows XP, network and printers. If you want to install the Bruker BioSpin NMR-SUITE on a PC which is already in use, you can skip this part and start with part two.

Note: You can also use the Bruker BioSpin NMR-SUITE 3.5 on Windows 2000!



Part two describes the installation and configuration of the NMR-SUITE and some necessary additional software package. It is recommended to follow the instructions step by step.

In the last part, you can find some additional information for working with Windows XP and the NMR-SUITE and also some tips for troubleshooting.

Note that all text-messages and graphics shown in this book are taken from the current version of the respective software products. Small differences to other versions are possible but generally speaking they should be very similar.

If you have any comments or suggestions, or if you find any errors in this manual, please do not hesitate to contact us at:

`nmr-software-support@bruker-biospin.de`

1.2 Conventions

Bold-Courier: Windows XP commands to be entered from the keyboard

Bold-Times: Windows XP commands, applications or buttons to be clicked with the mouse

Bold-Courier-Italics: NMR-SUITE commands to be entered from the keyboard

Bold-Times-Italic: NMR-SUITE commands to be clicked with the mouse

Courier: a file name or directory name

Courier Small Italics: response of the system

Courier Small: the contents of a file

Times italics: any name which is not a file name e.g. hostnames, usernames etc.

<>: place holder

1.3 Hardware and software requirements for NMR Suite

1.3.1 Special PC Hardware requirements

To run XWIN-NMR we recommend the following computer hardware:

- PC with CPU Clock ≥ 1 GHz
- Memory ≥ 512 MB
- Video (graphics)-card memory: 64 MB ¹
- Ethernet card (to control a spectrometer, it is essential to have a second ethernet card)
- Mouse with 3-button possibilities

If your hardware does not meet these requirements, XWIN-NMR might still run but with a much lower performance.

The Installation was tested on a 'hp workstation xw4100' PC with a 'NVIDIA Quadro4 380 XGL' graphics card and two 'Broadcom NetXtreme Gigabit Ethernet' cards.

1.3.2 Spectrometer requirements

XWIN-NMR 3.5 is released for datastations and Avance spectrometers. Systems that are working well with XWIN-NMR 3.0 or 3.1 do not need any hardware upgrade. Systems that are upgraded from XWIN-NMR ≤ 2.6 have to have at least the EC levels that are shown below.

Those hardware components that are not listed here are independent of a special software version and can be used with every NMR-SUITE version. If you have an older EC level, update to the most recent one (e.g. TCU3 actual EC level 29).

Please note that AQS and AQX/AQR components cannot be interchanged.

If your Avance spectrometer does not meet the above specifications, please get in touch with your local Bruker representative for your upgrade options.

1. It is recommend not to use shared memory graphics, because in some cases memory problems could be observed.

1.3.2.1 Avance systems with AQX/AQR rack

CCU:

The following EC levels are required for all spectrometers with Windows, they are not specific to XWIN-NMR 3.5.

<i>WINDOWS: the following EC levels are necessary</i>	
CCU 04 (part number H2552)	requires at least EC level 04
CCU 05 (part number H2570) EC level between 00 and 19	requires at least EC level 05
CCU 06 (part number H2570) EC level between 20 and 29	requires at least EC level 24
CCU 08 (part number H2570) EC level between 30 and 39	requires at least EC level 35
CCU 08 (part number H2570) EC level between 40 and 49	requires at least EC level 43
CCU 09 (part number H2570)	requires no specific EC level

• TCU

TCU 1 main board (part number H5811 or 5812)	requires at least EC level 03
TCU 0 main board (part number H2558)	requires at least EC level 07
TCU extention board (part number H2562)	requires at least EC level 03
	DMX and DRX with more than 5 channels: requires at least EC level 20

• RCU (Note: 'normal' RCUs and multiple receiver RCUs should not be mixed!)

RCU 1/1 (part number Z002488) 64 kB SRAM & 1MB DRAM	requires at least EC level 06
RCU 1/2 (part number Z012488) 256 kB SRAM & 2MB DRAM	requires at least EC level 06
RCU 1/3 (part number Z022488) 1 MB SRAM & 2MB DRAM	requires at least EC level 06

• **Multiple Receiver RCU**

RCU 1/4 (part number Z052488)	requires no specific EC level
RCU 2/4 (part number Z062488)	requires no specific EC level
RCU 3/4 (part number Z072488)	requires no specific EC level
RCU 4/4 (part number Z082488)	requires no specific EC level
RCU 1/5 (part number Z003206)	requires no specific EC level
RCU 2/5 (part number Z003207)	requires no specific EC level
RCU 3/5 (part number Z003208)	requires no specific EC level
RCU 4/5 (part number Z003209)	requires no specific EC level

• **FCU0**

FCU0: for use without cortab	requires at least EC level 04 64k-memory: part number H2556 256k-memory: part number H2554
FCU0: for DSX without use of cortab	requires at least EC level 05 64k-memory: part number H2556 256k-memory: part number H2554
FCU0: for use with cortab with EC level between 00 and 19	requires at least EC level 07 64k-memory: part number H2556 256k-memory: part number H2554
FCU0: for use with cortab with EC level higher than 20	requires at least EC level 22 64k-memory: part number H2556 256k-memory: part number H2554

- **Tomo FCU**

part number T5565 (64k memory) for use without cortab	requires at least EC level 00
part number T5565 (64k memory) for use with cortab	requires at least EC level 02
part number T6765 (256k memory) for use with or without cortab with EC level between 00 and 19	requires at least EC level 00
part number T6765 (256k memory) for use with or without cortab with EC level between 20 and 29	requires at least EC level 21

1.3.2.2 Avance systems with AQS rack

- **CCU 10**
 - *WINDOWS*: every EC level will work

- **FCU 3**

part number H5822 (64k memory)	requires no specific EC level recommended at least EC level 04
part number H9598 (256k memory)	requires no specific EC level recommended at least EC level 02

- **RCU** (Note: RCUs with EC level 06 of the AQX/AQR rack can be used also in a AQS rack)

RCU 1/2 (part number Z003678)	requires no specific EC level
-------------------------------	-------------------------------

- **TCU 3**

part number H5813 with EC level between 00 and 19	requires no specific EC level recommended at least EC level 09
part number H5813 with EC level between 20 and 29	requires no specific EC level recommended at least EC level 28

1.3.3 Software requirements



- Windows XP for NMR-SUITE ≥ 3.5
- NTFS filesystem on the partition where the NMR-SUITE is installed
(note that you can convert a FAT filesystem to NTFS, see chapter 4.1)
- NTFS filesystem on all partitions where XWIN-NMR data are stored
- Hummingbird NFS Server (for spectrometer control only) [see Chapter 10]
supported versions:
 - Version 7.1 (on CD: NT Toolkit 2 for NMR-SUITE)
- Hummingbird Exceed X Server [see Chapter 10]
 - Version 7.1.1 (on CD: NT Toolkit 2 for NMR-SUITE)
- Web Browser: Internet Explorer $\geq 6.x$ (*CD* or *WWW*) [see Chapter 7]
- Web Server e. g. Apache (on CD: NMR-SUITE for Windows 2000 / Windows XP) [see Chapter 8]
- Flexlm License Manager (on CD: NMR-SUITE for Windows 2000 / Windows XP) [see Chapter 12]
- PDF viewer (Bruker BioSpin recommends to use the Adobe Acrobat Reader) [see Chapter 11.5]

1.4 Important Windows XP functions and their shortcuts

The following Windows XP functions will be used regularly in this manual. They can all be started in different ways by mouse click or by entering a command on the keyboard. The following section describes some ways to start important functions:

1. Open the **Management Console**:
 - **My Computer** → right click **Manage**
2. Working as other User:
 - Right click on many icons → choose **Run as ...**
 - Right click in Explorer on many applications → choose **Run as ...**
 - Type in a command prompt:
runas /user:administrator cmd.exe
this will ask you for the administrator password and then open a Command prompt with administrator permissions
3. Open the Control Panel:
 - Click **Start** → **Control Panel**
 - Click **My Computer** → **Control Panel**
 - Press **Ctrl+Esc** → **s** → **c**
4. Open a Command Prompt:
 - Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
 - Press **Ctrl+Esc** → **r** → enter **cmd** → click **Enter**
5. Open the Task Manager:
 - Click the **RIGHT** mouse button on the Taskbar → click **Task manager**
 - Press **Ctrl+Shift+Esc**
6. Search for files or directories:
 - Click **Start** → **Search** → **For Files or Folders**
 - Enter **Ctrl+Esc** → **s** → **s** → click **Enter**
 - Press **F3** while the focus is on the desktop
(if the focus is not on the desktop: click on the desktop first)
7. Start the Windows Explorer:
 - Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
 - Right-click **Start** → **Explorer**
 - Double-click icon **My Computer** on the desktop
8. Configure the network:
 - Click **Start** → **Control Panel** → **Network Connections**

- Right-click **My Network Places** → **Properties**
9. Close a hierarchy of windows opened from **My Computer**:
- Press **Alt+Shift+F4**

More shortcuts may be found in chapter 18.3.1

Chapter 21.1 contains a blank list for important names and numbers of the hard- and software of your PC. It is recommended that you fill in the information there before you start the installation.

1.5 Important Windows configurations

This Installation Guide for the NMR-SUITE refers to the following configurations for Windows XP. Several functions (e. g. Control Panel, Start menu, Windows Explorer) can be configured in a *Classic view-mode* or *Category view-mode* (Windows XP style). These modes are not only different in style. They can be different in the way commands are entered.

1.5.1 Configure the Start Menu

For this manual the Start Menu is configured in the Windows XP style.

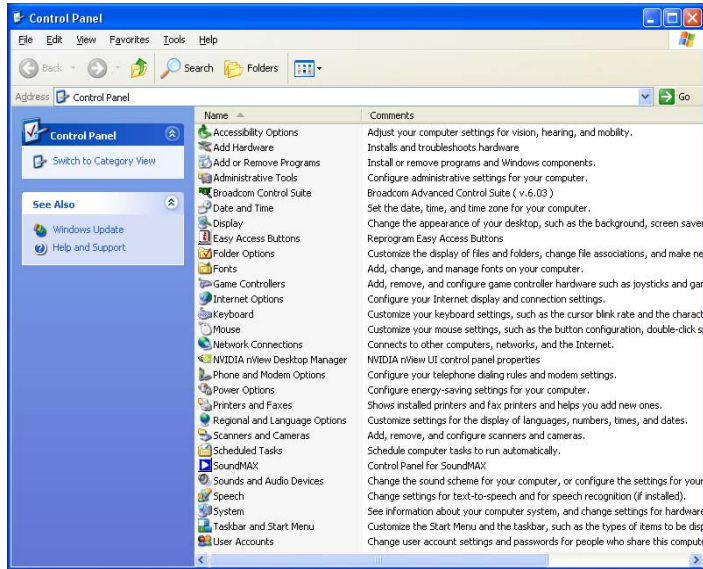
- Click the **RIGHT** mouse button on the Taskbar → click **Properties**
- Click **Start Menu** → click **Start Menu** → click **OK**



1.5.2 Configure the Control Panel and the Windows Explorer

For this manual the Control Panel and the Windows Explorer were configured in the *Classic View* style.

- Click on the left side on *Switch to Classic View*



Part I

Windows XP - Installation and Configuration

Chapter 2

Installation procedure

Before you start:

2.1 Do's and Don'ts under Windows XP

2.1.1 Do not re-install Windows XP

Not only will it usually not cure the problem, you also lose all additional pre-installed software (e.g. NMR-SUITE, Office package, user accounting, screen and network drives etc.). All of these, YOU will have to put back on manually. In such a case it is very important to have a backup of the essential files (see chapter 13.6 and 15.10). It will be many hours until you are back where you started. **If you have problems, use the Event Viewer and the other diagnostic tools to locate the problem and cure it within Windows XP.** If you think you need a re-install consider an 'Windows XP repair'. Use the Windows XP restore option (described in chapter 15.12) to repair Windows XP to the status of that restore point rather than doing a scratch install. Re-installing Windows XP is a last resort and you should have very good reason to do it.

2.1.2 Use Windows sharing rather than FTP

Under Windows you locate other computers in the network with Windows Explorer and then you can use **drag-and-drop multiple files and entire directo-**

ries. You can also connect to UNIX machines in that fashion using a tool on the UNIX side called 'samba'. Installation details are in the chapter 5.4.3. Nevertheless, in some cases FTP is still the easiest way to get a file quickly.

2.2 Installation order

A complete new installation on a PC connected to a spectrometer involves the following steps:

1. Installing Windows XP (see chapter 3.1)
2. Installing Windows XP Service Pack (see chapter 3.2)
3. Installing the Graphics driver (see chapter 3.3)
4. Configuring the Display colors and resolution (see chapter 3.4)
5. Installing Internet Explorer 6.x (see chapter 7)

Step 1 to 5 are normally already done by the manufacturer.

6. Configuring the network (see chapter 5)
7. Installing a printer (see chapter 6)
8. Configuring Internet Explorer 6.x (see chapter 7)
9. Installing and configuring the Web Server (see chapter 8)
10. Installing and configuring the Exceed X Server (see chapter 10)
11. Configuring the Exceed X Server (see chapter 10)
12. Installing the NFS Server (see chapter 10)
13. Installing the NMR-SUITE (see chapter 11.3)
14. Configuring the NFS Server (see chapter 11.6)
15. Installing the NMR-SUITE license (see chapter 12)
16. Configuring of the NMR-SUITE for spectrometer control (see chapter 13.1.1)
17. Installing a PDF viewer (see chapter 11.5)

If your PC is already in use, steps 1 to 6 are probably already done. In that case, you can start with step 6: the installation of the network. Some of the required programs may already be installed: click **Start** → **Programs** and look for:

- Exceed
- NFS Maestro Server

- Bruker BioSpin NMR-SUITE
- PDF viewer (Adobe Acrobat → Acrobat Reader <version-number>)

2.3 Removing existing software

Windows XP is more complex than you might think. Many files that are uploaded during an installation go into other parts of the system or replace existing versions of files. Thus, an uninstall is more like a build-back and you need that to really clean things out. By removing the directory, you don't solve your problem and also you lose the installation log which is stored as the software is installed. This log is very important and used by the uninstaller to make sure it finds every file that went on in the first place.

Use the uninstaller from Control Panel, i. e. the icon labeled 'Add/Remove Programs'.

Without a log this software will not work any more. See chapter 21.2 for a brief description.

If the NMR-SUITE is already installed and you want to install a new version or re-install the same version, you must first remove the old version and reboot the computer.

If you are running NMR-SUITE ≤ 2.5 you have to de-install as described in the following way; if you have version ≥ 2.6 the installation manager of the NMR-SUITE 3.5 CD-ROM will start the de-installation of the necessary programs automatically, after you have made your selection (see chapter 11.3).

Your own AU programs, pulse programs and parameter sets are NOT removed when you de-install XWIN-NMR. If you want to re-install any other package like Visual C++, NFS or Exceed, you must first remove that package (see below), reboot the computer and then re-install the package.



Never delete directories to remove a program

Always use the 'Add/Remove Programs' tool

Re-install a program in the following way:

→ remove the program → reboot → install the program → reboot

1. Click Start → Settings → Control Panel

2. Double-click the icon **Add/Remove Programs**

3. A window '*Add/Remove Programs*' will appear:

If you want to re-install the entire NMR-SUITE (see chapter 11.3), please remove the packages:

- | | |
|-----------------------------|----------------------|
| • Bruker: XWIN-NMR | Bruker: AURELIA/AMIX |
| • Bruker: XWIN-PLOT | Bruker: SBASE |
| • Bruker: ICON-NMR | Bruker: FLEXIm |
| • Bruker: DISKLESS | Bruker: NMR-CHECK |
| • Bruker: NMR-SIM | Bruker: NMR-GLP |
| • Bruker: NMR-SUITE patches | Bruker: NMR-GUIDE |

Note that not all of these packages are necessarily installed!

- Select the package that you want to remove
- Click the button **Change/Remove**
- A window '*Check Setup Information*' will appear
- Check if the path is correct then click **OK**
- A window '*Remove Programs From Your Computer*' will appear:
 - A growing bar shows the progress of the de-installation
 - When the de-installation is finished: click **OK**
- Repeat step b) to e) to remove further packages or click **OK** to close the window '*Add/Remove Programs*'

4. Close the window '*Control Panel*'

5. Reboot the computer.

During the installation of the NMR-SUITE, several entries are made in the Windows XP Registry. If an NMR-SUITE package, e.g. XWIN-NMR is removed as described above, the corresponding entry in the Registry is automatically deleted.

2.4 Autorun of installation programs

Many software packages like the NMR-SUITE as well as Windows XP support the Autorun feature. This means that the installation program automatically starts up when you insert the CDROM. This, however, only works if the Autorun is enabled. If it is not, nothing will happen after inserting the CDROM. In this case you can start the installation program as follows:

1. Click **Start** → **Settings** → **Control Panel**
2. Double-click the icon **Add/Remove Programs**
3. Click **Add New Programs** → **CD or Floppy**
4. A window '*Install Program from Floppy Disk or CD-ROM*' will appear:

The system is looking for a Floppy and/or a CD-ROM. If there are one of these the path will be shown in the field 'Open'

Click **Finish**

- 4a. If the field 'Open' is empty:
 - a) Click **Browse**
 - b) In the field 'Look in': select the CDROM drive
 - c) Find an icon **Setup** or **Setup.exe**
 - d) Click **Setup** or **Setup.exe**

or

1. Open the Windows Explorer
2. Select the path of the CDROM drive (normally D:)
3. Double click on the file `setup.exe`

The Administrator can re-enable Autorun by changing the Registry entry



Warning: You are about to edit the Windows Registry File. This is Windows XP's nerve center and errors in your setup may render your Windows XP installation UNUSABLE. Please make sure you have a recent Windows XP Repair Disk created BEFORE you proceed.

HKEY_LOCAL_MACHINE\SYSTEM\CurrentControlSet\Services\Cdrom\Autorun
from 0 to 1.

Chapter 3

Installing and configuring Windows XP Professional

Windows XP exists in two different forms: Windows XP Professional and Windows XP Home Edition.

The installation as described in this chapter is valid for the English version of Windows XP Professional on a hp workstation xw4100. In this case, you can install Windows XP exactly as described here. For other versions of Windows XP or other hardware, the installation procedure might be different.

For example, on some PC's the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

This description is intended for new installations. If Windows XP is already installed and you have problems:

Before you decide to re-install Windows XP, try to repair

Windows XP

Repairing Windows XP means that you selectively re-install parts of Windows XP, leaving application software and data intact.

3.1 Scratch install of Windows XP

1. If your computer is running:
 - a) Click **Start** → **Shut Down** → **Shut down the computer** → **Yes**
 - b) When you see the text '*It is safe to turn off your computer*' insert the CD-ROM '*Windows XP Professional*'.
2. Restart the computer and **Interrupt** the boot process by pressing the **F8** key.
(Do not press **F2** to go into *BIOS*, because there you can easily make your PC unable to boot.)
3. Wait until the boot device menu appears, select removable device with the **ARROW KEY DOWN** → **ENTER**
4. The '*Windows Setup*' screen appears:
 - a) You see at the bottom of the window '*Setup is loading files*'.
 - b) You see at the bottom of the window '*Setup is starting Windows XP*'.
5. A '*Windows XP Professional Setup - Welcome to Setup*' screen will appear with the Option of Continuing Setup, Repair a previous installation, or Quitting:
 - a) Press **ENTER** to Continue Setup.
6. A text about the "Windows XP Licensing Agreement" (EULA) screen will appear:
 - Press the **PGDN** key repeatedly until the end, press **F8** (to accept).
You see at the bottom of the window '*Searching for previous versions of Microsoft Windows*'.
7. If you have already other Windows XP installations on your PC, a list of them will occur. Press **ESC** in order to make a new installation instead of repairing an older one
8. If you have a couple of partitions on your hard disk, a list of currently available partitions will appear:
 - a) Press the **ARROW UP** or **DOWN** key to highlight the partition on which Windows XP must be installed.
 - b) Press **ENTER**
 - Select **Format the partition using the NTFS file system**, press **ENTER**

!

!

You are asked if you really want to format this partition or want to choose a different partition. After this point formatting will be started, **ALL DATA ON THIS PARTITION WILL BE LOST!** Data on other partitions (which might be on the same disk) remain untouched. If you want to format this partition, press **F** (to start formatting) and wait...

9. A window '*Your Computer will reboot in 15 s*' will appear

Remove any Floppy but keep the CD in its drive.

10. After the reboot the setup will continue automatically

A window '*Windows XP Setup*' occurs, please wait ...

11. A window '*Windows XP Professional Setup*' will appear:

- a) Click **NEXT** or wait for a short time
- b) Installing Devices (wait ...)
- c) '*Regional Settings*'
 - Normally you could leave English (United States) for system locale. Set the right keyboard layout → **NEXT**
- d) '*Personalize Your Software*'
 - Type in your name and organization → **NEXT**
- e) '*Your Product Key*' (see list in chapter 21.1):
 - Enter the **Product ID** which is specified on the manual '*Microsoft Windows XP Professional*' (on the Certificate of Authenticity) → **NEXT**
- f) '*Computer Name and Administrator Password*' (see list in chapter 21.1):
 - Enter the **Name** (hostname) you have chosen for your computer

Note that the first character must be alphanumeric and underscores are not allowed
 - Choose an Administrator password and enter it in the field **Password**, enter the same password in the field **Confirm Password** → **NEXT**

!

Important: remember the Administrator password.

- g) '*Date and Time Settings*'

- Check if Date&Time are set correctly, change if necessary
Select the correct time zone for your location, e.g.:

GMT + 01:00 for Germany
GMT - 05:00 for the US east coast
GMT - 08:00 for the US west coast

- click **NEXT**
 - h) '*Networking Settings*' (wait ...)
 - Enable Typical Settings → **NEXT**
 - i) '*Workgroup or Computer Domain*'
 - To get this information contact your system administrator, if you are not sure at the moment, please choose '*No, this computer is not on a network ...*' and enter the workgroup name → **NEXT**, please wait ...
 - j) The text '*Performing Final Tasks*' appears:
 - please wait ...
 - k) The text '*Completing the Windows XP Setup Wizard*' appears:
 - click **FINISH**, the system will reboot
 - l) Eject the CD-ROM
- 12.** A window '*Network Identification*' will appear → **NEXT**
- a) Users of this computer - who can log on to this computer?
 - Enable '*Users must enter a user name ...*', click **NEXT** → **FINISH**

You can log in as Administrator using the password which you have entered during the installation.

3.2 Installing Windows XP Service Pack

PCs from Bruker Biospin are delivered with the latest Service Pack available at the time of delivery. In contrast to Windows NT it is under Windows XP not necessary anymore to reinstall the service pack after e. g. configuring the network.

The Service Pack can be downloaded from www.microsoft.com or www.microsoft.de.

For installation just follow the given instruction on the screen.

3.3 Installing the Graphics driver

Hewlett Packard PC's from Bruker BioSpin are delivered with Graphics driver on the CD. If you do not have a floppy or a CD and want to install a newer driver, you can download a Graphics driver from the Web. Go to <http://h20000.www2.hp.com/bizsupport/TechSupport/Product.jsp?prodTypeId=43563>

The Graphics drivers are offered as self-extracting .exe files. Just download the file for your system, then click its icon and insert a formatted floppy. This way, you can create a new Graphics driver floppy.

The Graphics driver CD can be installed as follows:

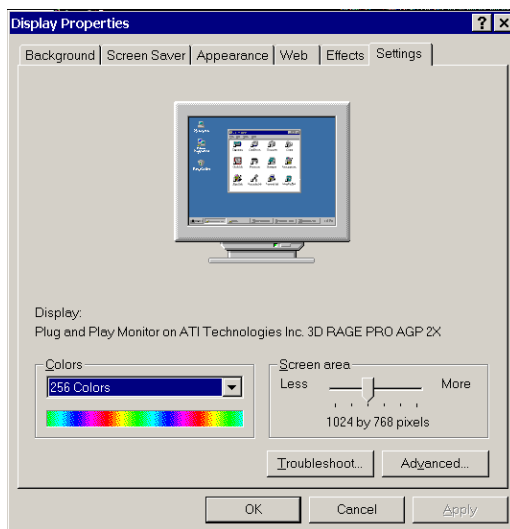
1. Insert the Graphics driver CD
2. Click **Start** → **Control Panel**
3. A window '*Control Panel*' will appear:
 - Double-click the icon **Display**
4. A window '*Display Properties*' will appear:
 - Click **Settings**
5. If the window 'Invalid Display Settings' appears: click **OK**
6. Click **Advanced** → **Adapter** → **Properties** → **Driver** → **Update Driver** → **Next** → enable '**Display a List ...**' → **Have Disk**
7. A window '*Install From Disk*' will appear:
 - a) Enter your CDROM, e.g. **d:** or accept the default if it is correct
 - b) Click **OK**
8. The Graphics driver which resides on the CDROM will appear: Click **OK**
9. A window '*Third-party Drivers*' will appear:
 - Click **Yes** (to proceed) and wait ...
10. A window '*Installing Driver*' will appear: click **OK**
11. In the window '*Upgrade Device Driver Wizard*': click **Finish**
12. Close the windows you have just opened
13. Remove the CD
14. A window '*Systems Settings Change*' will appear: click **Yes** (to reboot)

The procedure for other PC's or other Graphics drivers might be a little different.

3.4 Setting the Display Colors and Resolution

The NMR-SUITE requires a graphical resolution of 1024*768 or 1280*1024 with **256** colors. These values can be set in the following way:

1. Log in as Administrator
2. If a window '*Invalid Display Setting*' appears: click **OK**
3. Click **Start** → **Control Panel**
4. A window '*Control Panel*' will appear:
 - Double-click the icon **Display**



5. A window '*Display Properties*' which looks similar to the picture above will appear:
 - a) Click **Settings**
 - b) Click in the field **Colors**
 - If the value **256 Colors** is available:
 - Select **256 colors**
 - Continue with step c
 - If the value **256 Colors** is not available:

- Click **Cancel**
 - You must first install the Graphics driver for your Graphics card as described in chapter 3.3 and then set the display colors and resolution starting with step 1.
- c) Click in the field **SCREEN AREA** and select a resolution of **1024*768** or **1280*1024** (according to your preference).
 - d) Click in the field **Advanced** → **Monitor** → **REFRESH FREQUENCY** and select the maximum frequency for your monitor and the resolution selected in step c (check the documentation of your monitor). If you do not know this, just select one, e.g. **75 HZ** and see if it works (see step 6).
 - e) Click **Apply**
6. A window '*Default Monitor ...*' will appear
- a) Click **OK**
 - b) Answer the question '*Do you want to keep these Settings*' by clicking **Yes**
7. Click **OK** → **OK**

!

Important: If you do not test you might end up with a blank screen and no (easy) way back.

This color setting is mandatory and XWIN-NMR will not start if the colors are set to more than 256. You will get a message like:

```
CPR : Path to prog : "c:/Bruker/xwin-nmr/prog"
CPR : Path to exp ...                /exp"
CPR : Path to conf...                /conf"
CPR : waiting for FLEXlm license
CPR : Your FLEXlm license is valid until 16-may-2018
compare "source" with "dest" : 1 different colorcells
Graphics restart after normal error in Xlib
X Error of failed request: BadValue (integer parameter out of
range for operation)
Major opcode of failed request: 91 (X_QueryColors)
Value in failed request: 0xffffffff
Serial number of failed request : 1676
Current serial number in output stream: 1676
Program is exiting...
```

Chapter 4

Configuring Windows XP

4.1 Conversion of disk format from FAT to NTFS

Windows XP supports three file systems for fixed disks: FAT16, FAT32, and NTFS.

Bruker BioSpin XWIN-NMR and the datasets of the NMR experiments requires the file format NTFS. So if you want to use a FAT-partition of your harddisk(s) for installing the NMR-SUITE or storing NMR data you have to convert this partition to 'NTFS' (that is the file system of Windows XP) before you can install the NMR-SUITE. Only under NTFS, it is possible to have the file permissions, ownership and access management settings that make Windows XP secure. You can use the `convert` command `convert.exe` to convert an existing FAT volume to NTFS. Because this conversion retains all of your files (unlike a format operation), use `convert.exe` when you want to keep existing files on your volumes intact.

Before you convert a drive or partition to NTFS, consider the following:

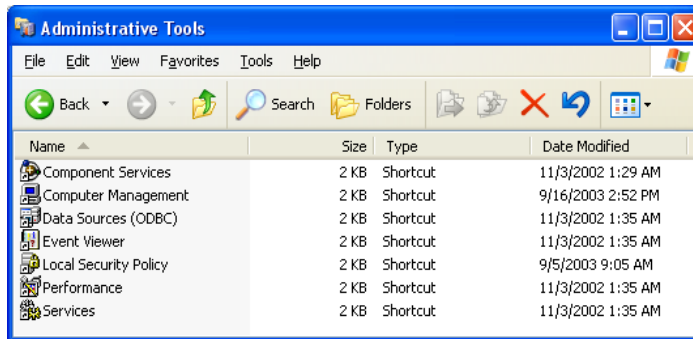
The conversion to NTFS is a one-way process. After you convert a drive or partition to NTFS, you cannot convert it back to FAT. To restore the volume to the previous file system, you must format it as FAT again. This action erases all existing data including your programs and personal files. In this case, you must either restore your data from a backup, or reinstall your operating system and programs.

`convert.exe` requires that you have a certain amount of free space on the drive or partition to convert it. If `convert.exe` determines that there is not enough free space on the volume, it does not convert the volume.

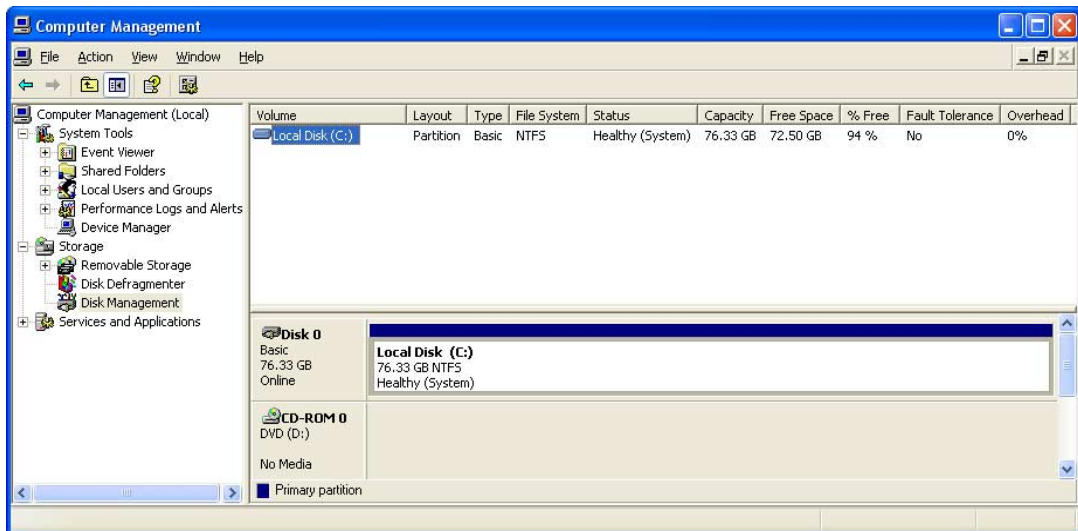
4.1.1 Check the Disk Partitioning

To check the configuration of the disk(s) of your PC, please start up the Disk Administrator utility from the command menus as shown below:

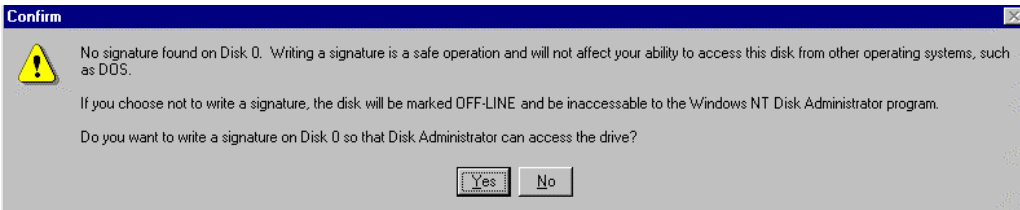
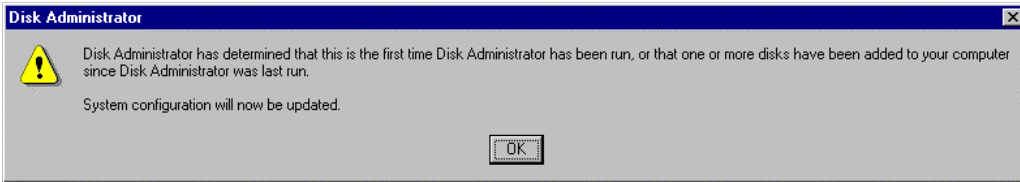
1. Click **Start** → **Control Panel** → **Administrative Tools**



2. Click on **Computer Management** → **Disk Management**



If this is the first time you start Disk Administrator, you probably see two information screens which you can confirm by clicking **OK**, respectively **Yes**:



Finally, the disk administrator will show you how many disk drives your system has, and how they are partitioned:

(Some PCs are delivered with one large partition C: that takes virtually all the space on the first disk).

Please realize that repartitioning the C: partition involves re-installing Windows XP!

Also, the maximum partition size with FAT is 4 GByte, with NTFS 7.8 GByte. Nevertheless, if you decide to make changes in the partitioning now is a good time to do it because you did not invest too much time in configuration and installation yet (e. g. the TOPSPIN is not installed and configured so far). All other partitions are usually empty at delivery of the PC and you can re-partition them or assign different drive letters.

An other file system format is FAT32 that has the advanced of none maximum partition size and that could be read by windows 9x, NT and 2000.

4.1.2 Converting partitions from FAT to NTFS

You see that in our case, both C: and D: already have the NTFS file system. If, on your system, partition D: or any other partition on which you want to store NMR

data is FAT, you can change that from the Disk Administrator. Just click

All Tasks → **Format** from the **Action** menu, select the NTFS file system and Start formatting.

Be aware that this will erase the entire partition.



The C: drive cannot be converted from the disk administrator. It can, however, be scheduled for conversion during the next boot up. In this way, the entire contents of C:, like Windows XP, will remain intact. Important: This is again a critical operation concerning power loss. If the conversion runs and the power goes away it will render the disk unusable and Windows XP must be re-installed. So it might be a good idea your PC to connect to an Uninterrupted Power Supply before you move on.

To convert a drive from FAT to NTFS without loss of data, start a Command Prompt from the command menus: Then type the following command on the command line and press return:

```
convert <drive:> /fs:ntfs
```

The system will ask you to schedule the actual conversion for the next boot-up and you will reply with 'y' as shown below:

```
Command Prompt
C:\>convert c: /fs:ntfs
The type of the file system is FAT.
Convert cannot gain exclusive access to the C: drive,
so it cannot convert it now. Would you like to
schedule it to be converted the next time the
system restarts (Y/N)? y
The conversion will take place automatically the next time the
system restarts.
C:\>
```

you do NOT need to re-boot now and wait the 2-3 minutes for it to complete. Just

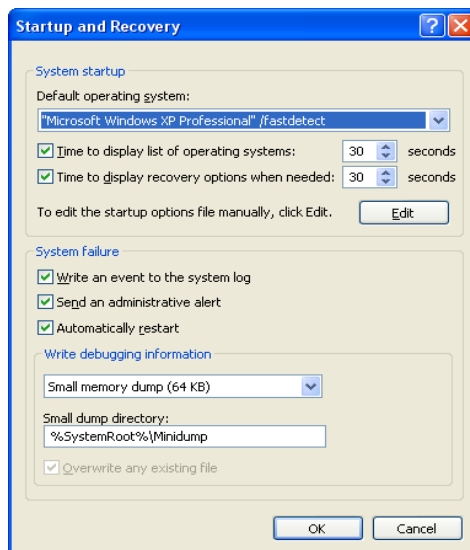
move on with the operations explained in the next chapter. The conversion to NTFS will automatically be done during the next re-boot.

4.1.3 Cutting down the re-boot time

1. Click **Start** → **Control Panel** → double click on **System**

A window 'System Properties' will appear:

2. Click **Advanced** → **Startup and Recovery**:



The default entry for the time the system waits for your boot selection during boot up is set to 30 seconds. You can set this entry to 5 seconds which is usually enough to select a different boot mode (or partition) if you want to do that.

3. Click **OK**

4.2 Bruker Service tools

Several tools for checking the spectrometer hardware are delivered with TOPSPIN. This includes tools for BSMS, HPPR, ACB, GRAD, HPCU, RX22. You can start a service tool as follows, for a full description see chapter 13.3:

1. Double-click the icon **Bruker Utilities** on the desktop
2. A window will appear with the icons Service tools, Test Tools etc.:
 - a) Double-click **Service Tools** to get a list of service tools
 - b) Double-click **Test Tools** to get a list of test tools
3. A windows with the available tools will appear:
 - Double-click any icon to start the corresponding tool

4.3 Windows XP Service Pack

All PC's delivered by Bruker BioSpin have the latest Service Pack installed. It can also be downloaded from the Microsoft Web pages www.microsoft.com or www.microsoft.de.

For installation just follow the given instruction on the screen.

Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

During the installation, you might get the message that files were detected which are not the original Windows XP files and which are also part of the Service Pack. Sometimes, these files are even newer than the ones in the Service Pack. This typically happens when you installed recent driver software. You are asked if these files should be overwritten. Bruker BioSpin recommends to answer this question with **No**, unless you are sure you want to update this file from the Service Pack.

Chapter 5

Windows XP Networking

- ! In order to run XWIN-NMR, you must setup the network (TCP/IP protocol), even if your PC is not connected to a spectrometer or to the laboratory network.¹ You can setup the network as a so-called Domain scenario or as Workgroup scenario. This chapter describes the Workgroup scenario.

5.1 TCP/IP configuration

This chapter describes how to install both the laboratory network (Workgroup scenario) and the spectrometer internal network for a 'hp workstation xw4100'. The description for other PC's with a different Ethernet card might be a little different. Before you start, make sure all network hardware components (network card, adapter, cables etc.) are properly connected. Then make a list of the following information:

- IP address for the PC in the laboratory network
- subnet mask of the laboratory network
- DNS domainname of the laboratory network
- IP address of the DNS nameserver(s) (if a nameserver exists)

1. The installation of the X Server Exceed requires an installed network. Furthermore, the XWIN-NMR license requires TCP/IP to be installed.

- IP address of the default gateway (if a default gateway exists)

If your PC is not physically connected to the laboratory network, you can use any IP address, subnet mask and domainname for the (external) network configuration. A frequently used IP address for such a 'standalone' computer is 192.168.0.1. This address is not assigned to any network computer (by world-wide-agreement). However, for the spectrometer internal network, you must use the values as specified below.

Perform the following steps according to the necessities of your setup:

5.1.1 Create a New Network Connection

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window *Network Connections* will appear
4. Click on *Create a new connection* on the left side of the window
5. A window *Network Connection Wizard* will appear → **NEXT**
6. Enable *Connect to the Internet* → **NEXT**
7. A window *Now Getting Ready* will appear
8. Enable **Connect using a broadband connection that is always on** → **NEXT**
9. A window *Completing the New Connection Wizard* will appear → Click **FINISH**

5.1.2 Configuring the TCP/IP of an existing Network Connection

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window '*Network Connections*' will appear
4. Highlight the connection you want to configure → **File** → **Properties**
5. Highlight the TCP/IP entry and click **Properties**
6. The window '*Internet Protocol (TCP/IP) Properties*' will appear:
7. Enable '*Use the following IP address*'
 - c) In the field **IP Address**: enter the IP address of your computer
 - d) In the field **Subnet Mask**: enter the subnet mask of your network

e.g. 255.255.255.0 or 255.255.0.0

- e) In the field **Default Gateway**: enter the IP address of the Default Gateway in your network (if available)
- f) If you have a nameserver:
 - In the field **Preferred DNS Server** enter the IP address of the nameserver
 - If you have a second nameserver enter his IP address in the field '*Alternate DNS server*'
- g) Click **Advanced** → **DNS**
- h) Enable the field **Append these DNS suffixes (in order)** → **Add**
 - In the window '*TCP/IP Domain Suffix*':
Enter the network domainname → **Add**
- i) Click **OK**
- j) If the question appears:
'This connection has an empty primary WINS address. Do you want to continue?' → **YES** → **OK** → **OK** → **CLOSE**

5.1.3 Configuring the TCP/IP of the Spectrometer Control:

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window '*Network Connections*' will appear
4. Highlight the connection you want to configure → **File** → **Properties**
5. Highlight the TCP/IP entry and click **Properties**
6. The window '*Internet Protocol (TCP/IP) Properties*' will appear:
 - In the field **IP Address**: enter **149.236.99.1**
 - In the field **Subnet Mask**: enter **255.255.255.0**

For the spectrometer network ONLY THESE VALUES ARE VALID!
Do not choose different settings for the IP address or Subnet mask.

 - Leave the Field Default Gateway empty
7. Click **OK**



If your PC controls a spectrometer we recommend to do the following:

1. Click **Start** → **Control Panel** → **Network Connections**
2. A window '*Network Connections*' will appear:
 - a) Select the Adaptor to which the spectrometer CCU is connected. This is normally, but not necessarily Adaptor 2.
 - b) Right mouse click → **Properties**
 - c) Disable the entry **Client for Microsoft Network (TCP/IP)** by clicking on the '+' sign to the left of the entry

5.2 Changing the hostname of the computer and its effects

If you want to change the hostname of your PC you can do this in the following way. IMPORTANT: You also have to change the text-file:



<XWINNMRHOME>\conf\nmrsuperuser

This file contains the computer-name and the Windows XP user which is the TOPSPIN-SUPERUSER. You can edit and change this file with a normal text editor like notepad if you are logged in as the Windows XP-user which is the NMRSUPERUSER.

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **Network Connections**
3. A window '*Network Connections*' will appear:
 - a) Click **Advanced** → **Network Identification**
 - b) A window '*System Properties*' will appear
 - c) Click **Network Identification** → **Properties**
 - d) In the field **Computer Name**: enter the new hostname

Note that the first character must be alphanumeric and underscores are not allowed!

- e) Click **OK**
4. A window '*Network Identification*' will appear:
 - Click **OK**
5. In the window '*System Properties*':

- Click **Close**
- 6. A window '*System Setting Change*' will appear:
 - Answer the question if you want to restart the computer now by clicking **Yes**
- 7. If you have *Floating* licenses you must change the hostname in the file `license.dat`. By default it resides in `C:\flexlm\Bruker\licenses`. You can do this in the following way:
 - a) Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
 - b) Enter: **cd c:\flexlm\Bruker\licenses**
 - c) Enter: **notepad license.dat**
 - Change the hostname in the **SERVER** line, then save and exit the file.

Of course, you can also change the license file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (hidden) extension `.txt` to the file `license.dat` which makes it unusable (see chapter 16.1.3).

5.3 Network diagnostic commands

Here is a list of the most important network diagnostic commands as they can be entered from the Command Prompt:

- **arp** - displays or modifies the IP to physical address translation tables
- **hostname** - displays the name of the current host
- **ipconfig** - displays information about the current TCP/IP configuration
- **netstat** - displays protocol statistics and current TCP/IP connections
- **ping** - checks if a destination host is receiving TCP/IP packets
- **route** - maintains and displays routing tables
- **tracert** - displays the route packets take to a destination host
- **net start** - displays all running services
- **net use** - display current network connection
- **nbtstat -a** - displays all registered NetBIOS names

5.4 Accessing remote files and directories

5.4.1 Sharing directories from a Windows XP host

Network operations under Windows XP primarily takes place via the Windows XP sharing mechanism. For example, you can share the data directory `c:\data` on *nthost_a* by taking the following steps:

1. Log in as Administrator on *nthost_a*
2. Open drive `C:` in the Explorer
3. Right-click on **data**
4. A popup window will appear:
Click **Sharing and Security**
5. A window '*Data Properties*' will appear:
 - a) Click **Share this folder**
 - Accept the default shared name *data*, or enter any other name ¹
 - Optionally, you can enter a comment
 - b) Optionally, you can set a user limit and/or shared permissions (note that the default permissions are Full Control for Everyone)
 - c) Click **OK**

The directory `c:\data` can now be accessed from any Windows XP host in the network, e.g. from *nthost_b*, in the following way:

1. Log in on *nthost_b* as normal user
2. Click the icon **My Network Places** on the desktop
3. A list of hosts in the network will appear:
 - Double-click the icon of *nthost_a*
4. A window '*Enter Network Password*' will appear:
 - a) In the field **Connect As:** enter the name of any user on *nthost_a*
 - b) In the field **Password:** enter the password for this user
→ A list of shared partitions/directories will appear

1. This is the name under which the directory can be accessed from other hosts

(The network password is only requested for the first connection).

Now you can:

- Access the remote directory as if it were local
- Copy the remote directory or any sub-directory or file in it, by dragging the corresponding icon into any target directory window (assuming you have the write permission in the target directory).

Note that the latter is only useful if the remote directory is not permanently shared.

5.4.2 Enabling and disabling Simple File Sharing

A PC under Windows XP Professional that is joined to a workgroup has the Simple File Sharing enabled by default. The Simple File Sharing is located in the folder's properties. When you set the Simple File Sharing the share and the file permissions are configured.

A Windows XP Professional PC that is joined to a domain use only the classic file sharing and security interface.

If you disable Simple File Sharing, the Shared Documents feature is not turned off.

You have more control over the permissions to individual users, if you disable the Simple File Sharing. However, you must have advanced knowledge of NTFS and share permissions to keep your folders and files secure.

!

It is recommended that you share folders only on the network within your user profile that remote users on other computers need to access. Never ever share the root of your system drive. In this case your computer is more vulnerable to malicious remote users.

To turn Simple File Sharing on or off:

1. Double-click **My Computer** on the desktop.
2. Click on **Tools**, select **Folder Options**.
3. Click the **View** tab, and then click to select the **Use Simple File Sharing (recommended)** check box to enable Simple File Sharing (click to clear this check box to disable this feature).

Levels of Access

There are five levels of access:

1. Level 1: My Documents (Private)
2. Level 2: My Documents (Default)
3. Level 3: Files in shared documents available to local users
4. Level 4: Shared Files on the Network (Readable by Everyone)
5. Level 5: Shared Files on the Network (Readable and Writable by Everyone)

In Levels 1, 2, and 3 folders are available only to a user who is logging on locally. Levels 4 and 5 folders are available to users who log on locally and remote users from the network .

You can have the following permissions:

Access Level	Everyone (NTFS/File)	Owner	System	Administrators	Everyone (Share)
Level 1	no	Full Control	Full Control	no	no
Level 2	no	Full Control	Full Control	Full Control	no
Level 3	Read	Full Control	Full Control	Full Control	no
Level 4	Read	Full Control	Full Control	Full Control	Read
Level 5	Change	Full Control	Full Control	Full Control	Full Control

1. Level 1: My Documents (Private)

Only the owner of the file or folder has the permission to read and write to the file or folder. All subfolders that are contained within a folder that is marked as private remain private unless you change the parent folder permissions. The option to make a folder private is only available to a user account in its own *My Documents* folder.

To Configure a folder and all of the files in it to Level 1:

- a) Right-click the folder → click **Sharing and Security**.
- b) Click to select the **Make this Folder Private** check box → click **OK**.

2. Level 2 (Default): My Documents (Default)

Only the owner of the file/folder and a local administrator have the permission to read and write to the file/folder. This is the default setting for all of the folders and files in each user's *My Documents* folder.

To configure a folder and all of the files in it to Level 2:

- a) Right-click the folder → click **Sharing and Security**.
- b) Ensure that both the **Make this Folder Private** and the **Share this folder on the network** check boxes are cleared → click **OK**.

3. Level 3: Files in Shared Documents Available to Local Users

Files are shared with users who log on to the computer locally. Local administrators and Power Users can read, write, and delete the files in the Shared Documents folder. Restricted Users can only read the files in this folder. In order to allow Remote Users to access folders/files at Level 3, you must share them out on the network (Level 4 or 5).

To configure a file/folder and all of the files in it to Level 3:

- a) Start Microsoft Windows Explorer
- b) Copy or move the file/folder to the Shared Documents folder under My Computer.

4. Level 4: Shared on the Network (Read Only)

For everyone on the network and local users (including the Guest account (if activated)) the files are shared to read. But they are not allowed to modify the contents. User that can connect to the computer on the network are able to read and change these files.

To configure a folder and all of the files in it to Level 4:

- a) Right-click the folder → click **Sharing and Security**.
- b) Click to select the **Share this folder on the network** check box
- c) Click to clear the **Allow network users to change my files** check box → click **OK**.

5. Level 5: Shared on the Network (Read and Write)

This level is recommended only for a closed protected network that has a fire-wall configured.

This level is the most available and least secure of all access levels. Any user can read, write, change, or delete a file in a folder shared at this access level.

To configure a folder and all of the files in it to Level 5:

- a) Right-click the folder → click **Sharing and Security**
- b) Click to select the **Share this folder on the network** check box → click **OK**.

NOTE: All NTFS permissions that refer to Everyone include the Guest account.

5.4.3 Sharing directories from a UNIX host using Samba

If you are logged in on a Windows XP host, you can access data which reside on a UNIX host, using the sharing mechanism. This, however, only works if the Samba package is installed on the UNIX host. Samba is available from <http://www.samba.org/samba/download.html>. Proceed as follows:

1. Download the correct version `samba53.*` or `samba6x.*` depending on your IRIX version (`uname -r`).
2. Install with `inst -f sambaxx.2.0.xx.tardist`
3. Within `inst` use `list` to show information about the package and `go` to install it.
4. After installation is done, you may configure it with the SWAT tool. This tool (Samba Web Administration Tool) is started, if you enter the address "`http://localhost:901/`" into your Web Browser. eg: **Toolchest** → **Internet** → **Open Web Browser**.
 - define the **workgroup** in the **GLOBALS** section
 - the **directories** you want to share in the **SHARES** section
 - and the password encryption settings. The default is **no** (see chapter 20.4.3), but Windows XP is sending encrypted passwords by default so you have to change it in Samba or in Windows XP (see step 7)
5. You will find an actual description of the current samba version and the corresponding installation in:

<ftp://ftp.bruker.de/pub/nmr/binaries.indy/samba-x.readme>

More information on setting up samba, password encryption and many other features of Samba can be found in:

`/usr/samba/docs`

6. Reboot the UNIX host
7. If the Samba on the UNIX host is configured as `'encrypt passwords = no'` (check it in the SWAT) and you want this configuration, you must enable plain passwords on your PC. You could do that as follows *but be aware that this would create a security leak (see chapter 20.4.3)*:
 - a) Log in as Administrator
 - b) Get the file:
`/usr/samba/docs/WinXP_PlainPassword.reg`
from the UNIX host, e.g. with FTP
 - c) Execute this file by clicking on its icon in the Explorer
 - d) Reboot the PC

5.4.4 Mounting Windows XP partitions from a UNIX host using NFS

If your PC is controlling a spectrometer, installation of the Hummingbird NFS Server is mandatory. The partition `C:\Bruker\Diskless\clients\spect` is mounted via NFS by the spectrometer CCU (which is a UNIX host). In the same way, you can mount any Windows XP partition or directory on any UNIX host. Proceed as follows:

1. Export the Windows XP partition as described in chapter 11.7.1. In step 4, you must enter the partition and, optionally, the UNIX host(s) to which it must be exported.
2. On the UNIX host:
 - a) Open a UNIX shell
 - b) Type `su` to become superuser
 - c) Create a mount directory, e.g. `mkdir /ntdata`
 - d) mount the partition, e.g.:
 - on SGI: `mount nthost:/c/data /ntdata`
 - on X32: `mount -f NFS nthost:/c/data /ntdata`

Note that, if the pathname on the Windows XP hosts contains uppercase letters, these must also be specified with the mount command.

Important: on a SGI with IRIX 5.*, XWIN-NMR cannot read data which reside on an NFS mounted WindowsNT/2000 partition. This is an error in Hummingbird NFS Server 5.14 and is fixed with version 6.1 with the configuration as NFS2. The problem does not occur with IRIX 6.*.

5.4.5 FTP

Network transfer under Windows XP is generally done via the directory sharing as described in chapter 5.4.1 and 5.4.3. Nevertheless, Windows XP supports transfer via FTP. Just enter '**ftp hostname**' from a Command Prompt and you can transfer files.

5.4.6 Transferring single files with FTP

1. Click **Start** → **All Programs** → **Hummingbird Connectivity V7.1.1** → **Host Explorer** → **FTP for Windows**
2. The window '*FTP*' will appear.
3. A window showing the directory tree on the local host will appear
4. A window '*Open Connection*' will appear.
 - a) In the field **Server Name**: enter the name of the remote host, e.g. *wombat*
 - b) In the field **User Name**: enter your username, e.g. *john*
 - c) In the field **Password**: enter your login password
 - d) Click **Open**

Note that you can also log in as any other user if you know the password.

5. In the window '*FTP*' you will see two windows:
 - The directory tree on the local host. Here you can select files which you want to **put** on to the remote host.
 - The directory tree on the remote host. Here you can select files which you want to **get** from the remote host.

Click an icon (file or directory) to select it for transfer. If you double-click a directory icon, the directory will be opened and its contents will appear.

6. In the window '*FTP*':

- Click **File**
Depending on whether you selected a local or a remote file for transfer, the command **get** or **put** will be available. Click one of them to start the transfer.
- 7. A window '*Get*' or '*Put*' will appear:
 - a) In the field **To**: enter the destination name and directory
If you leave this field empty the file will be copied under the same name to the directory displayed in the title bar of the directory window.
 - b) Click **OK**
- 8. If you want, you can store the connection to the remote host for later usage:
 - a) Click **File** → **Save As**
 - b) In the field **File name**: enter any name, e.g. *wombat_john*
- 9. Close the FTP session by clicking **File** → **Exit**
- 10. In a later FTP session you can open the this connection by clicking:
 - **File** → **Open**
 - Double-click the entry *wombat_john.fs*

5.4.7 Transferring directory trees with FTP

The Hummingbird Exceed FTP program allows you to transfer directory trees. Note that this is very unusual in a Windows environment because network transfer usually takes place via sharing (see chapter 5.4.1 and 5.4.3). However, if you want to transfer a directory tree you can do this in the following way:

1. Create a text file, e.g. with **notepad**, with the following contents:

```
gettree /u/data/guest/nmr/dataname
```
2. Perform step 1 to 4 as described in chapter 5.4.6.
3. In the window '*FTP*':
 - Click **Tools** → **Load FTP Command Script File**
4. A window '*Load FTP Command Script Files*' will appear:
 - a) Click in the Field **Look in** and find the directory in which you stored the text file (see step 1).
 - b) The text file will appear: click it
 - c) Click **Open** (to start the transfer)

5.4.8 Telnet

Windows XP contains a **telnet** command for remote login. Just enter **telnet hostname** in a Command Prompt to login to a remote host. The telnet command can only be used to login from your PC to a remote host (e.g. a UNIX host) but not vice versa.

With Windows XP it is also possible to do a telnet login to a Windows XP computer but this feature is not very convenient.

5.5 Requirements for the 'Send' function in XWIN-NMR

Alternatively to printing and faxing diagnostics results to Bruker BioSpin or somewhere else, you can send the same information via electronic mail. For this to work, the spectrometer PC needs access to the Internet, i.e. to an Internet gateway in your local network. If the Personal Computer has not yet been set up for e-mail transmission proceed as follows:

Install a program that allows for composing and sending e-mail messages. If you have **Microsoft Internet Explorer 6.0** or newer, we recommend to install it. Internet Explorer is bundled with an e-mail application called **Outlook Express**. Outlook Express is perfect for NMR-CHECK's and XWIN-NMR's e-mail features.

The description how to use the send button in XWIN-NMR is found in the 'XWIN-NMR processing manual'

5.5.1 Installation and configuration of Outlook Express

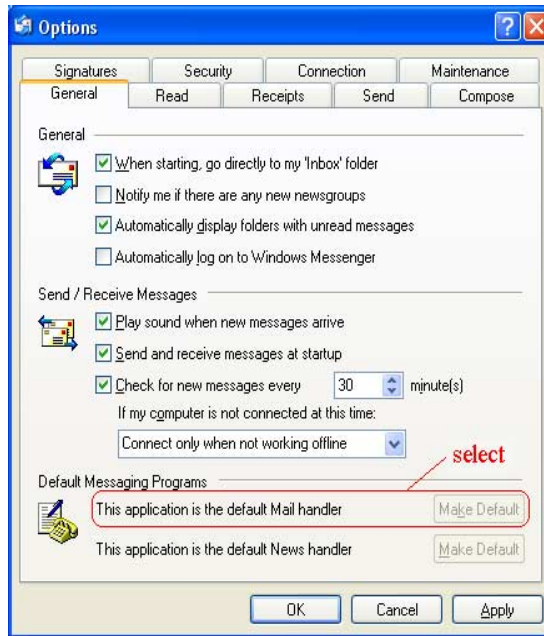
Outlook Express gets automatically installed with Microsoft Internet Explorer 6.0 or newer.

- Open **Start** → **All Programs** → **Outlook Express**
- or double-click the **Outlook Express** icon on the desktop.

Supply all parameters asked for by the setup wizard. Contact your network administrator if you are not sure what to fill in.

Select **Options** from Outlook Express' **Tools** menu and configure the General Set-

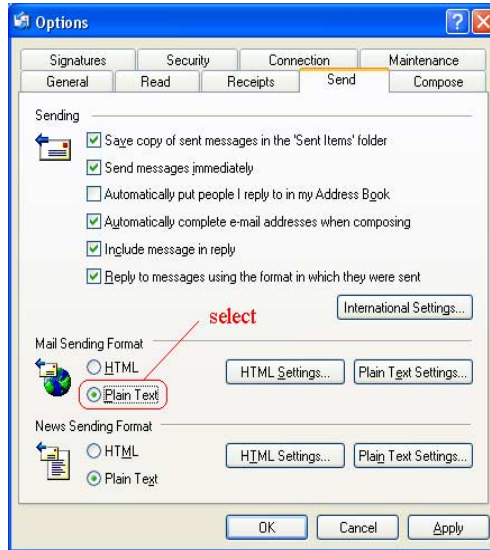
tings as shown below.



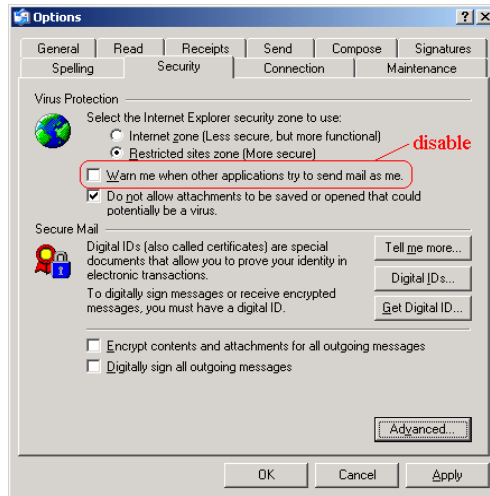
Outlook Express version 6 is able to handle the default mail handling and the simple MAPI client as one. It is sufficient to enable the setting as default mail program

Do not reboot the computer now. Open the **Options** interface again, switch to the

Send page and select the topics as shown below.



Switch to the **Security** page and disable *Warn me when other applications try to send mail as me*, then reboot the computer.



To disable this warning might be a security leak. If you do not disable this warning, you get a warning every time if ICON-NMR send an e-mail.

5.5.2 Sending an e-mail with Outlook Express

Fill in the correct recipient's address.

Click the **Send** button.

If you want to use an e-mail application not mentioned here, make sure it has some 'use as simple MAPI client' feature and activate it.

5.6 Installing the NMR Suite in a Windows XP Domain

Windows XP provides two different security scenarios for computer networks, the Workgroup and the Domain scenario. With a Workgroup scenario, each computer has its own local security database of user accounts and passwords. This means that users from workstation A are not known at workstation B. They might have the same name on both workstations but internally they are represented by two different security identifiers. Users from workstation A can access files on workstation B via the sharing mechanism (see chapter 5.4.1). The Workgroup scenario is typically used for small networks. For large networks, the Domain scenario is usually preferred. In this case, one computer (the Domain Controller, DC) maintains the security database for an entire group of Windows XP Computers. A Domain user can log on at each workstation in the Domain with a single account and password. Furthermore, the Domain Administrator's account has administration rights on every computer in the Domain. Nevertheless, a local Administrator account exists on each computer for local administration tasks.

The Bruker BioSpin NMR-SUITE fully supports both security scenarios. The description of the NMR-SUITE installation in chapter 11.3 is valid for a Workgroup scenario. This chapter describes the additional installation steps which are required for a Domain scenario. The NMR SuperUser (see chapter 11.1.1), which is specified during the installation of the NMR-SUITE can now be a local account or a Domain account¹. In both cases the NMR SuperUser only needs standard access permissions. The installation of the NMR-SUITE, however, requires Administrator rights because certain system services and two user groups are installed. Furthermore:

the NMR-SUITE must be installed as local Administrator

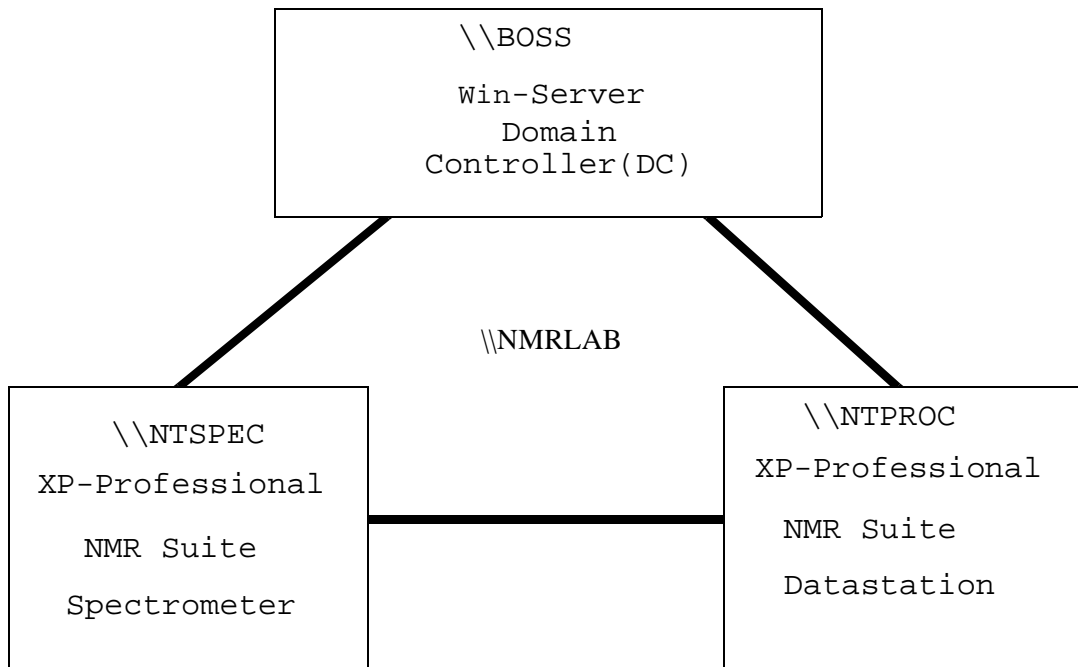
1. A Domain NMR Superuser is only supported in XWIN-NMR 2.6 or newer.

This means no Domain-wide administrative tasks are done during the installation.

The installation of the NMR-SUITE in a Domain involves the following steps:

1. Make sure that there is a Local or Domain account for NMR Superuser, or create one.
2. Installation of NMR-SUITE by the local Administrator.
3. Creation and configuration of global groups of NMR users by the Domain Administrator.
4. Make sure that all nmr users have an existing HOME directory

As an example, we use a Domain `\\NMRLAB` with two workstations; `\\NTSPEC` which controls a spectrometer and `\\NTPROC` which is used for processing. The security database resides on the Domain Controller `\\BOSS`. Step 2, the installation of the NMR-SUITE is the same on `\\NTSPEC` and `\\NTPROC` so it will only be described for `\\NTSPEC`.



5.6.1 Creating an NMR SuperUser account

Before you install the NMR-SUITE, you have to make sure that there is an account for NMR SuperUser. If there is none which you like to use, create a new one. According to your preference this can either be a local or a Domain account.

5.6.1.1 Creating a local NMR SuperUser account

If you prefer a local NMR Superuser, do the following:

1. Log on at Windows XP Professional Workstation \\NTSPEC as the local Administrator or any other user who has User Administration rights, selecting \\NTSPEC as Domain.
2. Open the User Manager and create an account for the NMR SuperUser, e.g. with the name *nmrsu*. (see also chapter 11.1.1 and 14.1).

5.6.1.2 Creating a Domain NMR SuperUser account

If you prefer a Domain NMR SuperUser, do the following:

1. Log on at the Domain Controller \\BOSS as the Domain Administrator.
2. Open the User Manager and create an account for the NMR Superuser, e.g. with the name *nmrsu* (see also chapter 11.1.1 and 14.1).

Note that the installation of the NMR-SUITE, which must be done as local Administrator, relies on the fact that the NMR SuperUser was correctly installed. It cannot check if a Domain NMR SuperUser really exists.

5.6.2 Installing the NMR Suite

The installation of the NMR-SUITE involves the following steps:

1. Log on as local Administrator on Windows XP Professional \\NTSPEC.
2. Install the NMR-SUITE as described in chapter 11.3.

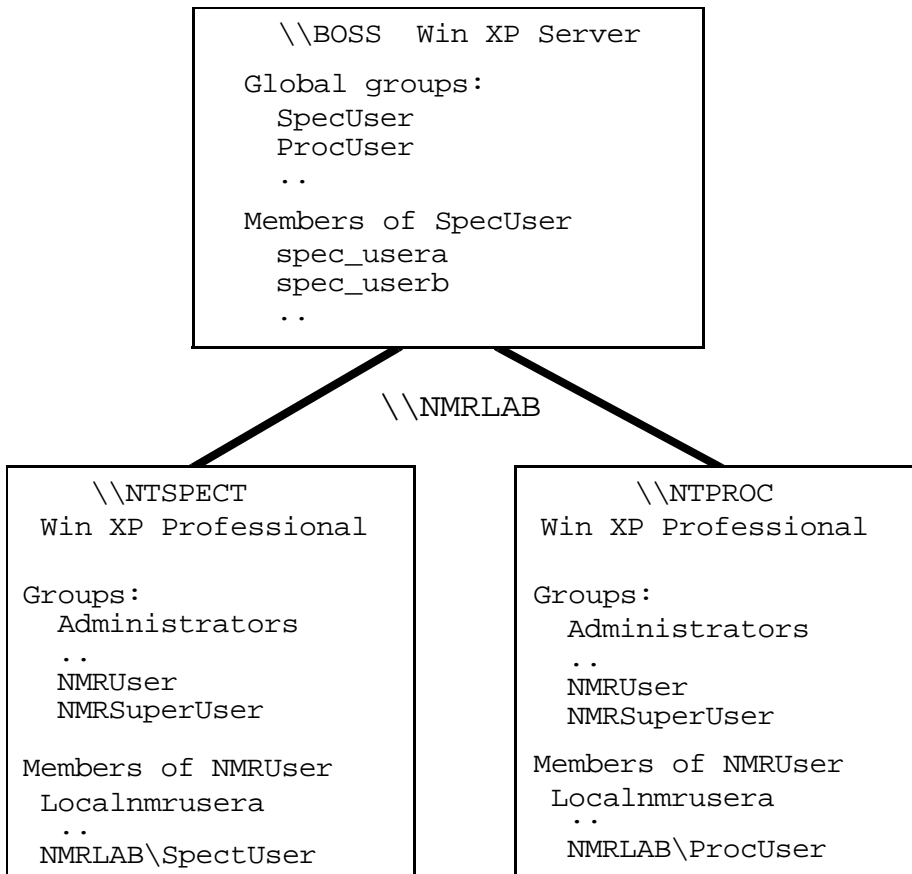
During the installation process, you will be asked for the NMR SuperUser. Enter the name of the NMR SuperUser account as created before (see chapter 5.6.1).

After the installation process, NMR users cannot start the NMR-SUITE yet. First they must be added to the local group NmrUser. Users with a local account, e.g. localnmrusera can simply be added to NmrUser as described in chapter 14.1.3. However, for users with a Domain account, which is typical in a Domain scenario,

we recommend to use global groups as described in chapter 5.6.3.

5.6.3 Installing global user groups

The NMR-SUITE installation program creates a local group NmrUser. Each user who wants to use the NMR-SUITE must be a member of this group. Domain users could be added individually to the local group NmrUser but, in a network with many Workstations and varying users, this would be an elaborate task. Therefore, we recommend to create so called global user groups. Global groups are created by the Domain Administrator on the Domain Controller. Each global group contains users who are allowed to do certain tasks, e.g. start XWIN-NMR on a specific spectrometer or datastation. These global groups are then added to the local group NmrUser on the various Workstations in the network. In our example, the Domain Administrator creates the global groups *SpecUsers* and *ProcUsers* which are then added to the local group NmrUser on `\\NTSPEC` and `\\NTPROC` respectively. After that, for example, the global user `spec_usera` can control the spectrometer from Workstation `\\NTSPEC`. By managing these global groups on the Domain Controller, the Domain Administrator can control which users can use the spectrometer and which can use the datastation. In practice, one global group will be added to the local group NmrUser on several Workstations and NmrUser on one Workstation can contain several global groups.



The installation of the global user groups involves the following steps:

1. Log on at the Domain Controller as Domain Administrator.
2. Create the global groups *SpecUser* and *ProcUser*.
3. Log on as local Administrator at workstation *\\NTSPEC*, selecting *\\NTSPEC* as Domain.
4. Add the global group *NMRLAB\SpecUser* to the local group *NmrUser* as described in chapter 14.2.4.
5. Repeat step 3 and 4 for *\\NTPROC* adding *NMRLAB\ProcUser* to the local group *NmrUser*.

5.6.4 Check for the HOME directory of every nmr users

There are two possibilities for the HOME directory of an user, local on every PC or fixed on one PC in the domain. Bruker supports both scenarios, the last one is a little bit more convenient, because the resource file (used by command 'setres') of Xwin-nmr is stored in the home directory of the user. If there are individual settings it is easier to have to create this file only once and use it on all Xwin-nmr installations of the windows domain.

Note that the configuration of the NMR-SUITE relies on the fact that the given HOME directory of an user exists. The HOME directory cannot be created by XWIN-NMR.

Chapter 6

Installing a Printer

Printers must be installed at a Windows XP level and can then be used in XWIN-NMR and XWIN-PLOT.

6.1 Installing a new local printer

Installing a local printer implies installing the software, e.g. the printer driver for that printer. You can get printer drivers from various sources:

1. From a CDROM or floppy which was delivered with the printer:
Please follow the instruction in the printer installation guide. If you do not have one, just insert the floppy or CDROM. The *Setup* program might start automatically. If it does not, open the Explorer and find a file named Setup or Install and click it.
2. From the Web:
Just go to the manufacturers Web home page, e.g. www.hp.com, www.canon.com or www.epson.com and look for **Download** or **Drivers**. Usually, an executable file can be downloaded which can be unpacked and installed, simply by clicking on it.
3. From the Windows XP CDROM:
If you do not have a CDROM or floppy with printer software and no Web access you can install a printer driver from your Windows XP CD. You will get

a list of printers for which a driver was available at the time your Windows XP version was released. If your printer type does not appear, you can select a related printer. However, Bruker BioSpin does not guarantee that this will work (see chapter 6.1.1 for installation instructions). Note:

Bruker BioSpin does not supply printer drivers for Windows XP!

6.1.1 Installing a printer from the Windows XP CDROM

A large number of printer drivers are available on the Windows XP CDROM. Note that these are the drivers which were available at the time Windows XP was released. For older printers these are usually valid. For newer printers the drivers might not be on the CD or better drivers might be available. Please use drivers delivered with the printer or from the Web whenever possible.

You can install a printer from the Windows XP CD as follows:

1. Log in as Administrator
2. Click **Start** → **Printers and Faxes**
3. A window '*Printers*' will appear:
 - Double-click the icon **Add Printer**
4. A window '*Add Printer Wizard*' will appear: → Click **NEXT**
 - a) Click **Local Printer**, enable **Plug and Play** search mode if you want that the system looks for a new printer → Click **Next**
 - b) A window '*New Printer Detection*' will appear
 - if the system finds a right printer → Click **Next**
 - if the system does not find a printer define it manually during the next steps → Click **Next**
 - c) Select the port to which the printer is connected → Click **Next**
 - d) In the field **Manufacturers:** select the manufacturer of the printer, e.g. HP
 - e) In the field **Printers:** select the type of the printer

If your printer does not appear in the list, select a related printer type or click **Cancel** and get the driver from the Web.
 - f) Click **Next**
 - g) In the field **Printer Name:** enter the name under which you want to use the printer (or accept the default name)

h) If other printers are already installed, you will be asked if the new printer must be the default printer:

- If you want to use this printer as default printer → Click **Yes**
- If you do not want to use this printer as default printer → Click **No**

i) Click **Next**

j) '*Printer Sharing*': Do one of the following:

If the printer must be available for other computers in the network:

- Click **Shared**
- In the field **Share Name**: enter the name by which the printer can be accessed from a remote host, e.g. *viola_deskjet*
- Click **Next**
- A window '*Location and Comment*' appears. Write in some informations about the location, the printer administrator and individual printer specifications (e. g. the fax-default-printer etc.) → Click **Next**.

If this printer should only be used on the local computer:

- click **Not shared**.

k) Click **Yes** (to print a test page) → Click **Next** → Click **Finish**

5. If the window '*Insert disk*' appears:

- Insert the CDRom '*Windows XP Professional*' → Click **OK**

6. A window '*Files Needed*' will appear:

- Click **OK** (to copy the Driver files for your printer from the CD)

7. A new icon will appear in the window '*Printers*' (see step 3):

- a) Click the right mouse button on the new printer's icon
- b) Click **Printing Preferences** in the pop-up menu

8. A window '*Printing Preferences*' will appear:

- a) Click **Advanced**
- a) Click in the Field **Paper Size**
- b) Select the correct paper size for your printer
- c) Click **OK** → **OK**

Step 8 makes sure that applications like Word, Excel, Paint and TOPSPIN ... will use this paper size as default.

6.2 Remote printing from a PC to a PC

6.2.1 On the PC to which the printer is physically connected

If the printer is not installed yet:

- Install the printer as described in chapter 6.1. During this installation you have to choose between 'shared' and 'not shared'; click **Shared**

If the printer is already installed as a local printer:

- a) Log in as Administrator
- b) Click **Start** → **Printers and Faxes**
- c) Click the right mouse button on the printer icon and select **Sharing ...**
- d) A window '*<printer name> properties*' will appear:
 - Click **Shared**
 - In the field **Share Name**: enter the name under which the printer can be accessed on the network, e.g. *viola_deskjet*
 - Click **OK**
- e) Close the window '*Printers*' by clicking the **X** button

6.2.2 On the PC from which you want to print

1. Click **Start** → **Printers and Faxes**
2. A window '*Printers*' will appear:
 - Double-click the icon **Add Printer**
3. A window '*Add Printer Wizard*' will appear:
 - a) Click **Network printer**
 - b) Click **Next**
 - c) A window '*Locate your printer*' will appear, enable one of the three fields under the point '*What Do You Want To Do*'
 - '*Find a Printer in the Directory*' is a powerful search tool that is looking for a printer with the properties you want in the active directory if you are member of domain
 - Click **Next**, a window '*Find Printers*' will appear:

- Choose the domain path in the field '*In*'
- In the menu '*Features*' you have the possibility to enable some additional search modes like resolution, paper size etc.
- Click **Find Now**
- '*Type the Printer Name ...*'
 - Use this option if you already knows whats the name of the printer you want to install (use the form `//<Print-Server>/<Printer-Name>`) or if you want to start a search in the subdomain of your network
 - Click **Next**
- '*Connect to a Printer ...*'
 - Use this option if you want to connect to a internet printer that has an own URL address



Wait until list of shared printers on that UNIX host appears. If this list does not appear within one minute, click the **Network Connections** icon on the desktop and try to connect to the remote host. Then go back to the window '*Connect to printer*', click the remote host again and see if get a list of shared printers now.

4. The window '*Add Printer Wizard*' will appear:

- a) Do one of the following:
 - Click **Yes** if you want to use this printer as default printer
 - Click **No** if you do not want to use this printer as default printer
- b) Click **Next**, click **Finish**

6.3 Remote printing from a UNIX host to a PC

6.3.1 On the PC to which the printer is physically connected

Install the printer as described in chapter 6.2.1.

1. Log in as Administrator
2. Insert the CDROM '*Windows XP Professional*'
3. Close the window '*Windows XP CDROM*' by clicking **Exit**
4. Click **Start** → **Control Panel** → **Network Connection**

5. A window '*Network and Dial-up Connection*' will appear:
 - Click on the pull down menu **Advanced** → **Optional Network Component**
6. A window '*Optional Network Component*' will appear:
 - Enable **Other Network File and Print Services**
 - Click on **Networking Services** to highlight it then click **Details**
 - enable **Simple TCP/IP Services** → **OK**
 - The check box for **Other Network File and Print Services** is now white and that one for **Networking Services** grey and both have a tick, click **Next**
7. Click **Start** → **Settings** → **Control Panel** → **Administrative Tools** → **Services**
8. A window '*Services*' will appear:
 - a) Scroll down and check the following entries:
 - Simple TCP/IP Services
 - Print Spooler
 - TCP/IP Print Server

If one of these entries is set to **manual**:

 - Click that entry to highlight it
 - Click **Action** → **Properties** → **Startup type** → select **Automatic** → **OK**
9. Click **Start** → **Shut Down** → **Restart the computer** → **Yes**

6.3.2 On the UNIX host from which you want to print

On the UNIX host, you must setup a network printer as follows:

1. Open a UNIX shell
2. Become superuser; type **su**
3. Edit the file `/etc/printcap` and make an entry like:

```
laserjet|HP :\
:rm=viola.netx.applic.com:\ 1
:rp=hplj4ml:\
:sd=/usr/spool/lpd/hplj4ml:\
```

1. Depending on your network you must enter hostname or hostname.domainname

```
:sh:
```

where:

- *laserjet* is the name for the printer on the UNIX host
- *viola.netx.applic.com* is the hostname.domainname of the PC
- *hplj4ml* is the name of the printer on the PC

4. Create the spooling directory which is specified in `/etc/printcap`:

- a) `mkdir -p /usr/spool/lpd/hplj4ml`
- b) `chown daemon.daemon /usr/spool/lpd/hplj4ml`
- c) `chmod 770 /usr/spool/lpd/hplj4ml`

More information on network printing under UNIX can be found in the manual `netprint` which is available on:

<http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html>

and as '*Network Printing*' in the XWIN-NMR online help.

6.4 Remote printing from a PC to a UNIX host without Samba

Remote printing from a PC running Windows XP on a printer connected to a UNIX host can be realized in two different ways:

- by installing the Microsoft TCP/IP Printing package on the PC
- by installing Samba on the UNIX host (see chapter 6.5)

The first method is easier to install. The second method has advantages if you also want to use Samba's capability to share UNIX directories with Windows XP hosts.

6.4.1 Configuring the PC from which you want to print

1. Log in as Administrator
2. Insert the CDROM '*Windows XP Professional*'
3. Close the window '*Windows XP CDROM*' by clicking **Exit**
4. Click **Start** → **Control Panel** → **Administrative Tools** → **Services**
5. A window '*Services*' will appear:

Do you see an entry Microsoft TCP/IP Printing?

Yes? → Click **Cancel** and continue with step 6.

No? → Go to chapter 6.3.1

6. Click Start → Printers and Faxes

7. A window 'Printers' will appear:

- Double-click the icon **Add Printer**

8. A window 'Add Printer Wizard' will appear:

- a) Click **Next** → **Local Printer**, disable '**Automatically detect and install my Plug and Play Printer**', click **Next**
- b) Enable **Create New Port** select Type **LPR Port** → **Next**

9. A window 'Add LPR compatible printer' will appear:

- a) Enter the name of the LPD server (the UNIX host)
- b) Enter the name the printer has on the UNIX host¹
- c) Click **OK**
- d) Close the window '*Printer Ports*' by clicking **Close**

10. In the window 'Add Printer Wizard':

- a) Click **Next**
- b) In the field **Manufacturers**: select the manufacturer of your printer
- c) In the field **Printers**: select your printer type
- d) Click **Next** (to accept the default printer name)
- e) Click **Not shared** → **Next** → **Finish**
- f) Answer the question '*Was the test page printed correctly?*' with **Yes**
- g) Close the windows '*Printers*' and '*Control Panel*' by clicking the **X** button

6.4.2 Configuring the UNIX host to which the printer is physically connected

1. Open a UNIX shell
2. Become superuser; type **su**
3. Edit the file `/etc/printcap` and make an entry like:

```
laserjet|HP :\  
:lp=/dev/plp:\  
:sd=/usr/spool/lpd/laserjet:\
```

1. You can check this name by logging in on the UNIX host and entering '`lpstat -t`'


```
:sh:\  
:sf:
```

where:

- `laserjet` is the name for the printer on the UNIX host
- `lp` is the port where the printer is physically connected

4. Create the spooling directory which is specified in `/etc/printcap`, e.g.:

- a) `mkdir -p /usr/spool/lpd/laserjet`
- b) `chown daemon.daemon /usr/spool/lpd/laserjet`
- c) `chmod 770 /usr/spool/lpd/laserjet`

5. Edit the file `/etc/hosts.lpd` and enter two lines like:

```
viola  
viola.netx.applic.com
```

where *viola* is the hostname and *netx.applic.com* the domainname of the remote PC.

6.5 Remote printing from a PC to a UNIX host with Samba

This chapter describes how you can install a printer on a Windows XP computer, when the printer is physically connected to a UNIX host, e.g. an SGI. The method described here involves the installation of Samba, which also allows you to access directories on the UNIX host from the Windows XP host. Alternatively, you can install the printer without using Samba, as described in chapter 6.4.

6.5.1 Configuring the UNIX host to which the printer is physically connected

1. Get the Samba package from the Internet and install it as described in chapter 5.4.3.
2. In the SWAT (see chapter 5.4.3) choose the printer according to your preference. All Printer that are defined in the `printcap` occurs in the pop-up menu.
3. Reboot the UNIX workstation

6.5.2 Configuring the PC from which you want to print

1. Click **Start** → **Printers and Faxes**
2. A window '*Printers*' will appear:

- Double-click the icon **Add Printer**
3. A window '*Add Printer Wizard*' will appear:
- a) Click **Network printer**
 - b) Click **Next**
 - c) A window '*Locate your printer*' will appear, enable one of the three fields under the point '*What Do You Want To Do*'
- '*Find a Printer in the Directory*' is a powerful search tool that is looking for a printer with the properties you want in the active directory if you are member of domain
 - Click **Next**, a window '*Find Printers*' will appear:
 - choose the domain path in the field '*In*'
 - In the menu '*Features*' you have the possibility to enable some additional search modes like resolution, paper size etc.
 - Click **Find Now**
 - '*Type the Printer Name*'
 - use this option if you already know the name of the printer you want to install (use the form //*<Print-Server>/<Printer-Name>*) or if you want to start a search in the subdomain of your network
 - Click **Next**
 - '*Connect to a Printer ...*'
 - Use this option if you want to connect yourself to a internet printer that has an own URL address

Wait until list of shared printers on that UNIX host appears. If this list does not appear within one minute, click the **My Network Place** icon on the desktop and try to connect to the remote UNIX host. Then go back to the window '*Connect to printer*', click the remote UNIX host again and see if get a list of shared printers now.

- Double-click the printer connected to the UNIX host, e.g. **laserjet**
4. A message about a missing NULL printer driver will appear:
- Click **OK**
5. A window '*Add Printer Wizard*' will appear:

- a) In the field **Manufacturers**: select the manufacturer of the printer, e.g. **HP**
- b) In the field **Printers**: select the type of the printer
If your printer does not appear in the list, select a related printer type or click **Cancel** and get the driver from CDROM or from the Web.
- c) Click **Next**
- d) If other printers are already installed, you will be asked if the new printer must be the default printer:
 - If you want to use this printer as default printer: click **Yes**
 - If you do not want to use this printer as default printer: click **No**
- e) Click **Next**, click **Finish**

6.6 Installing a printer with a JetDirect print server

If your printer is connected to the network via a HP JetDirect print server, you must install it in the following way:

1. Log in as Administrator
2. Install the Service Microsoft TCP/IP Printing as described in chapter 6.3.1.
3. Click **Start** → **Printers and Faxes**
4. A window '*Printers*' will appear:
 - Double-click the icon **Add Printer**
5. A window '*Add Printer Wizard*' will appear:
 - a) Click **Next** → **Local Printer**, disable '**Automatically detect and install my Plug and Play Printer**', click **Next**
 - a) Enable **Create New Port** select Type **LPR Port** → **Next**
6. A window '*Add LPR compatible printer*' will appear:
 - a) In the field **Name or Address of server providing lpd**: enter the name or IP address of the Print Server.
 - b) In the field **Name of printer or print queue on that server** you must enter:
 - **raw1** if you have an internal JetDirect adapter
 - **raw1**, **raw2** or **raw3** if you have an external JetDirect print server, depending on the JetDirect port to which the printer is connected.

- c) Click **OK**
- 7. In the window '*Printer Ports*':
 - Click **Close**
- 8. In the window '*Add Printer Wizard*':
 - Click **Next**
- 9. Continue the installation as described in chapter 6.1.1, step 4d.

Part II

NMR-Suite Installation and Configuration

Chapter 7

Installing Internet Explorer

7.1 When do I need Internet Explorer?

If you want to use the NMR-GUIDE which is part of TOPSPIN, it is necessary to install *Internet Explorer* version ≥ 6.0 . It is available on the *Windows XP CDROM*.

If you use Windows XP, you should install Service Pack 1.

7.2 Is the Internet Explorer 6.0 or newer already installed?

Before you install *Internet Explorer* ≥ 6.0 you should check whether it is already installed:

1. Login as Administrator
2. Click **Start** → **All Programs** → **Internet Explorer**
3. A window *Microsoft Internet Explorer* will appear
4. Click **Help** → **About Internet Explorer**
5. A window *About Internet Explorer* will appear
6. Is the *Version* entry 6.0 or more
 - *Yes?*

A correct version of the *Internet Explorer* is already installed, you can go to the configuration in chapter 7.4

- *No?*

There is not a correct version of *Internet Explorer* installed, please follow the instructions in chapter 8

7.3 Update of Internet Explorer

1. Click **Start** → **All Programs** → **Internet Explorer**
2. A window *Microsoft Internet Explorer* will appear
3. Type in the address:
<http://www.microsoft.com/windows/ie/default.asp>
4. Click on **download** and follow the instructions

7.4 Configuration of Internet Explorer

1. Click **Start** → **All Programs** → **Internet Explorer**
2. A window *Microsoft Internet Explorer* will appear
3. Click on **Tools** → **Internet Options** → **Advanced**
4. Ensure that the following Settings are enabled:
 - Java console enabled (requires restart)
 - Java logging enabled
 - JIT compiler for virtual machine enabled (requires restart)
5. Restart your computer

Chapter 8

Installing the Web Server for using NMR-GUIDE

8.1 When do I need a Web Server?

If you want to use the NMR-GUIDE, which is part of the NMR-SUITE, it is necessary to install a web server first.

8.2 Which Web Server is necessary

Bruker recommends the Apache web server, which is available either on the NMR-SUITE CD or on the web (<http://httpd.apache.org>) because the IIS [(Internet Information Service), part of the Microsoft Windows CD] is often attacked by hackers and viruses and so could be a security problem.

If you currently use the IIS only for running NMR-GUIDE, then you can switch to the Apache web server. Before doing so, contact your system administrator to be sure that no other applications which require the IIS are running. If you are in doubt about this, you can use both web servers at the same time (see chapter 8.4.4).

8.3 Installation of Apache web server

8.3.1 How to install Apache web server

If it is already installed, the previous configuration will not be changed, the configuration information for NMR-GUIDE will just be added. You can download the Apache Web Server from the web:

<http://httpd.apache.org>

Or you can install it from the NMR-SUITE CD. On the CD go to the directory
windows/apache

and execute the file

apache_1.3.27-win32-x86-no_src.msi

8.4 Configuration of Apache web server

8.4.1 Situation 1 - no WWW server running

1. Before you install NMR-GUIDE you have to install the Apache Web Server.

You can follow the default installation.

Only three parameters are required during the installation

- Name of the computer (e. g. donna)
- The domain name of the computer (e. g. software.testfirm.de)
- The email address of the Web administrator

2. Check the Apache server with a WWW browser, type in the URL:

<http://localhost/>

You should see the Apache server's default page.

3. Now you can install the NMRGuide.

During the NMRGuide installation two lines will be appended to the file:

C:\Program files\Apache Group\Apache\conf\httpd.conf

These lines are:

NMR-Guide - include

Include C:/Bruker/<XWINNMRHOME>/guide/java/apache-NT4W2K/ht-tpd.conf

4. After the installation, the Apache server SERVICE should be stopped and restarted.
5. To test NMRGuide, open Internet Explorer and type in the URL:
http://localhost/guide/test.html

8.4.2 Situation 2 - Apache web server already running.

Follow steps 3 - 5 of chapter 8.4.1.

8.4.3 Situation 3 - Switching from IIS to Apache web server

1. Go to the services menu
2. Stop the IIS service.
3. Disable the IIS server.
4. Follow steps 1 - 5 of chapter 8.4.1

8.4.4 Situation 4 - Running Apache web service while running IIS

1. Go to the services menu
2. Stop the IIS service.
3. Follow steps 1 - 3 of chapter 8.4.1
4. Find the following line in the Apache's httpd.conf file:

Port 80

Replace it with

Port 8080

5. Go to Services.
 - Start the Apache server.
 - Start the IIS server
6. To test the IIS server, open Internet Explorer and type in the URL:
http://localhost/
7. To test the Apache server, open Internet Explorer and type in the URL:
http://localhost:8080/

8. To test the NMRGuide, open Internet Explorer and type in the URL:

http://localhost:8080/guide/test.html

8.4.5 Secure Apache web service configuration

The standard configuration of the Apache web server has a security hole, which is caused by the httpd.conf file. Due to the security hole, the computer can be mis-used for sending out massive numbers of mails.

The security hole can be easily fixed. Please add the following lines to the httpd.conf file from the NMR-GUIDE distribution. The httpd.conf is located:

<XWINNMRHOME>\guide\java\apache-NT4W2K

You should add the following four lines after the four "Alias" lines in the httpd.conf file.

----- Start of block to be inserted in httpd.conf for Apache 1.3 versions -----

<Directory proxy:>*

Order Deny,Allow

Deny from all

Allow from localhost

</Directory>

----- End of block to be inserted in httpd.conf for Apache 1.3 versions -----

Similarly, add the following lines for Apache 2.0.

----- Start of block to be inserted in httpd.conf for Apache 2.0 versions -----

*<Proxy *>*

Order Deny,Allow

Deny from all

Allow from localhost

</Proxy>

----- End of block to be inserted in httpd.conf for Apache 2.0 versions -----

To make the change effective, you must reboot your computer. Alternatively, you can go to the Services menu (Control Panel) and stop and start the Apache web server there. That way you will not have to reboot your computer.

The "Allow from localhost" restricts the use of the NMR-GUIDE to your local computer. If you still want to use the NMR-GUIDE over the network, you may write something like "Allow from .your-localdomain.com". Actually, you can still use the NMR-Guide over the network. Only the dynamically generated table of contents on the left-hand side of the browser window will disappear. This is because the security patch will prohibit the access to the local proxy server.

If you want to test whether the fix works, do the following. Once you have modified the httpd.conf and restarted the Apache server, you open your browser and load

http://localhost

This should work. Next, open

http://localhost/guide/manualw.html

This should also work. Finally, go to another computer in your network, open a web browser and enter:

http://the_computername_where_NMR_Guide_is_installed/guide/manualw.htm

This should give you the page, but an error message should appear on the left-hand side along the lines of "access is denied".

Chapter 9

Compiling AU programs

XWIN-NMR is delivered with the free GNU *gcc* compiler.¹

It is installed automatically during installation of XWIN-NMR. With XWIN-NMR 3.5 it is no longer necessary to have the compiler Microsoft Visual C++ (the default compiler of XWIN-NMR < 3.5) installed.

So the default situation is that you can skip this chapter, because you do not need any special compiler installation or configuration.

9.1 Why does XWIN-NMR need a compiler?

XWIN-NMR only needs a compiler for compilation of AU programs. If you do not use AU programs, you do not need a compiler!

9.2 How can I use Microsoft Visual C++ if I want to?

If, however, Microsoft Visual C++ (version 6.0 or .Net) is installed on your system, you can configure XWIN-NMR to use it instead of the GNU compiler, for this you have to change the file:

1. If you like to work with the '*vi*' in Bruker's GNU shell, it is necessary to start it with the command '*vim*' in this version of the GNU package.

```
<XWINNMRHOME>\exp\stan\nmr\au\makeau
```

find the line:

```
# $opt_native = 1;
```

and remove the '#' so that the line becomes:

```
$opt_native = 1;
```

9.3 Problems with the default GNU compiler

Generally, the GNU compiler works properly with XWIN-NMR. However, if you have a second copy of `cygwin1.dll`, apart from the one delivered with XWIN-NMR, you might run into problems. If this happens you will get the following error message:

You have multiple copies of cygwin1.dll on your system.

*Search for cygwin1.dll using the Windows Start -> Find/Search facility and delete all but the most recent version. The most recent version *should* reside in x:\cygwin\bin, where 'x' is the drive on which you have installed the cygwin distribution*

If you have a problem like this you can remove the second copy of `cygwin1.dll` (not the one delivered with XWIN-NMR).

Chapter 10

Installing Exceed / NFS Server

10.1 NT Toolkit CD / NT Toolkit 2 CD

The Bruker BioSpin NT Toolkit CDROM CD (for Windows NT 4.0) contains:

- Hummingbird Exceed X Server 6.0.1 and
- Hummingbird NFS Server 5.1.4

Both versions do not support Windows XP.

Bruker BioSpin offers the new Bruker BioSpin NT Toolkit 2 CD for Windows 2000 and Windows XP that contains:

- Hummingbird Exceed X Server 7.1.1 and
- Hummingbird NFS Server 7.1

10.2 Preparing for the NT Toolkit installation

Bruker BioSpin NT Toolkit 2 CDROM (Windows 2000 and Windows XP) contain Hummingbird Exceed X Server and Hummingbird NFS Server. You must install the Exceed X Server in order to run XWIN-NMR (XWIN-NMR graphics are based on X11 functions). The NFS Server is required if your PC controls a spectrometer; it

makes the DISKLESS package available for the CCU. Hummingbird Exceed and NFS are available on the Bruker BioSpin NT Toolkit CDROMs or can be purchased from Hummingbird ¹.

Before you install the NFS Server:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- Enter **ipconfig /all**

and check if the network is installed. If it is not, install the network as described in chapter 5.

10.3 Installing the X Server Exceed

Currently supported versions for Windows XP of the X Server Exceed is 7.1.1: If this is already installed, you can skip this chapter.

If another version is installed, remove it according to chapter 2.3, reboot the computer and continue with chapter 10.3.1.

The description of chapter 10.3.1 refers to the installation of Exceed 7.1.1 from the Bruker BioSpin NT Toolkit 2 CDROM.

If you have the Hummingbird Exceed CD, be aware of the following. If it says Evaluation on the CD, it will only work for a limited amount of time. Please check if your delivery contains another Exceed CD. If it does, this is probably the full version. If it does not, you probably ordered an Evaluation CD. Please use the full version if you have one!

10.3.1 Installation of Exceed 7.x

The installation description is given for the version 7.1.1 but is also valid for all exceed versions 7.x.

1. Log in as Administrator
2. Insert the CDROM '*NT Toolkit 2 for NMR-SUITE*' or the Exceed CD from Hummingbird.
3. Double-click the icon **My Computer**
4. A window '*My Computer*' will appear:

1. See www.hummingbird.com

- Double-click the CDROM icon
- 5. A window showing the contents of the CDROM will appear:
 - Double-click **setupX** or **setupX.cmd**
- 6. A window '*Hummingbird Exceed V7.1.1*' will appear:
- 7. Click **Install Exceed**
 - a) This window will show the subtitle '*Installation type*'
 - Click **Personal Installation**
 - b) A window '*Choose Setup language*' will appear:
 - Choose **English (USA)** (you can choose any language you like, but this description is written for the English one)
 - Click **OK**
 - c) A window '*Hummingbird Setup Wizard*' that displays several progress bars will appear and finally show:

The Hummingbird Setup Wizard will install Hummingbird Exceed on your computer

 - Click **Next**
 - d) A window '*License Agreement*' will appear:
 - Click **I accept ...**
 - Click **Next**
 - e) A window '*Customer Information*' will appear. Insert the appropriate information or leave the proposals unchanged (it is important that this application will be installed for anyone who uses this computer):
 - Make sure that for the feature '*Install this application for:*' the field *Anyone who uses this computer (all users)* is enabled
 - Click **Next**
 - f) A window '*Destination Folder*' will appear:
 - Click **Next**
 - g) A window '*Setup Type*' will appear:
 - Click **Typical**
 - Click **Next**
 - h) A window '*Ready to Install the Program*' will appear:

- Click **Install**
- i) A window '*Installing Hummingbird Exceed*' will appear showing a progress bar
- j) A window '*Keyboard Preference*' will appear:
 - Click **Next**
- k) A window '*Xconfig Password*' will appear:
 - Insert a password and click **Next**
- l) A window '*X server tune up*' will appear:
 - Click **Next** (this procedure will take several minutes)
- m) A window '*Hummingbird Setup Wizard Completed*' will appear:
 - Click **Finish**
- 8. Back in the window '*Hummingbird Exceed V7.1.1*' :
 - Click **Back**
 - Click **Exit**
- 9. Remove the CDROM

10.3.2 Configuring of Exceed 7.x

The configuration description is given for the version 7.1.1 but is also valid for all exceed versions 7.x.

1. Log in as Administrator
2. Click **Start** → **All Programs** → **Hummingbird Connectivity V7.1.1** → **Exceed** → **Xconfig**
3. Enter the Xconfig password if it is requested, click **OK**
(this is the password that was entered during the installation of Exceed)
4. A window '*Xconfig*' will appear:
 - a) Double-click the icon **Keyboard Input**
 - A window '*Keyboard Input*' will appear
 - If necessary, select your keyboard by clicking the arrow at the right of the field **Primary**
 - Click **OK**
 - b) Double-click the icon **Mouse Input**

- A window '*Mouse Input*' will appear:
 - unselect **Middle Button Emulation**
 - Click **OK**
- c) Double-click the icon **Screen Definition**.
- A window '*Screen 0*' will appear:
 - Click **Common Settings**
 - If necessary, select **click** in the field **Native Window Manager Focus Policy** by clicking the arrow to the right of this field.¹
 - Unselect the item **Close Warning On Exit**²
 - Click **Screen 0**
 - Check the setting of **Server Visual**; for XWIN-NMR it must be set to **PseudoColor**
 - Click **OK**

NOTE: If Exceed 7.x is used under Windows XP with native display instead of an 8-bit mode, there are some bugs described in the Bruker BioSpin bug database. A possible workaround is to configure the following:

- d) Double-click the icon **Performance**
- Set *Default Backing Store* to **When Mapped**
 - Set *Maximum Backing Store* to **When Mapped**
 - Click **OK**

5. Close the windows '*Xconfig*'

6. To start Exceed 7.1.1 automatically with XWIN-NMR it is necessary to define the path where Exceed is located.

!

- Click **Start** → **Control Panel** → **MKS Toolkit**
- In the upcoming window click on the field **NutC4 Options**
- In the field **Category** select **X Windows system settings**
- In the field **X Server settings** click on other and browse for the path of exceed.exe, default path is:

C:\Program Files\Hummingbird\Connectivity\7.11\Exceed\exceed.exe

1. This means the XWIN-NMR window will get the focus when you click on it.

2. Otherwise you will always get a warning when closing XWIN-NMR or any sub-window.

- Click **OK**

10.4 Installing NFS Server



IMPORTANT:

- before installing NFS you must configure TCP/IP (see chapter 5.1)
- If your installation fails with following error message:

```
CreatThisService::Createservice:Error # [997]
```

Your network-adapter has no link to the network. Establish a link to the network or install the

NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:

- a) Click **Start** → **Control Panel** → **Network Connections** → Right-click **Local Area Connection xxx**
- b) Click **Properties** → **Install...** → **Protocol** → **Add**
- c) The *Select Network Protocol*-menu will appear after some seconds. → Click **NWlink ...** → **OK**
- d) After some seconds the Properties-menu will reappear: → Click **Close**

Currently supported version of the NFS Server for Windows XP is 7.1: If this one is already installed, you can skip this chapter.

If another version is installed, remove it according the chapter 2.3, reboot the computer and install a newer version.

Chapter 10.4.1 describes the installation of the NFS Server 7.1 from the Bruker BioSpin NT Toolkit 2 CDROM.

If you have the Hummingbird NFS Maestro CD be aware of the following. An Evaluation CD, will only work for a limited amount of time. Please check if your delivery contains another NFS Maestro CD. If it does, this is probably the full version. If it does not, you probably ordered an Evaluation CD. Please use the full version if you have one! Now insert the NFS Maestro CD.

10.4.1 Installing NFS 7.1.1 from Bruker BioSpin NT-Toolkit 2 CD

1. Log in as Local Administrator

2. Insert the CDROM '*NT Toolkit 2 for NMR-SUITE*'
3. Double-click the icon **My Computer**
4. A window '*My Computer*' will appear:
 - Double-click the CDROM icon
5. A window showing the contents of the CDROM will appear:
 - Double-click the icon **setupNFS** or **setupNFS.cmd**
6. A window '*Hummingbird Master Setup*' will appear:
 - Click **Install NFS Maestro Server**

This window will change to the subtitle '*Installation Type*'

- Click **Personal Installation**
- A window '*Chose Setup Language*' will appear:
 - Choose **English (USA)** (you can choose any language you like, but this description is written for the English one)
 - Click **OK**
- A window '*Hummingbird Setup Wizard*' will appear and display several progress bars. Finally it shows:

The Hummingbird Setup Wizard will install Hummingbird NFS Maestro Server on your computer ...

 - Click **Next**
- A window '*License Agreement*' will appear:
 - Click **I accept ...**
 - Click **Next**
- A window '*Customer Information*' will appear. Insert the appropriate information or leave the proposals unchanged (it is important that this application will be installed for anyone who uses this computer):
 - Click **Next**
- A window '*Destination Folder*' will appear:
 - Click **Next**
- A window '*Setup Type*' will appear:
 - Click **Typical**
 - Click **Next**
- A window '*Ready to Install the Program*' will appear:

- Click **Install**
- A window '*Installing Hummingbird NFS Maestro Server*' will appear showing a progress bar
- A window '*Hummingbird Setup Wizard Completed*' will appear:
 - Click **Finish**
- Back in the window '*Hummingbird Master Setup*':
 - Click **Back**
 - Click **Exit**

7. Remove the CDROM

Two certificates '*Proof of license*' are delivered with each CD '*NT Toolkit for NMR-SUITE*'. They prove that you have an official copy of the Hummingbird Exceed and NFS Server. Please keep these two certificates!

10.5 Configuring the NFS Server for spectrometer control

Before you can configure the NFS Server (described in chapter 11.6) you must first install the NMR-SUITE CDROM, particularly the DISKLESS package (see chapter 11.3).

Chapter 11

Installing the NMR Suite

11.1 Preparing for the NMR Suite installation

Before you install the NMR-SUITE:

1. Before you proceed, make sure you are logged in as Administrator. If you are not sure about this, press **Ctrl-Alt-Del** (just as for a logon). The upcoming screen tells you the current user-id. If you are indeed logged in as Administrator, click **Cancel**. Otherwise click **logoff** and then log on as Administrator.
2. Click **Start** → **Control Panel** → **System**
and check if Windows XP, Windows 2000 or Windows NT 4.0 Service Pack ≥3 is installed (see also chapter 3.1).
3. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
enter: `ipconfig /all`
and check if the network is configured. If it is not, configure the network as described in chapter 5.
4. Click **Start** → **All Programs**
and check if you see the entry Exceed. If this do not appear, you must install this package as described in chapter 10 respectively.
Exceed is required to run XWIN-NMR.

5. As a Local Administrator click **Start → Control Panel → Administrative Tools → Computer Management → Services and Applications**

and check if you see the entry Apache web service. If it not appear and you want to run the NMR-GUIDE you must install it as describe in chapter 8.

6. Click **Start → Control Panel → Display → Settings**

and check if the **Color Palette** is set to **256** and the **Desktop Area** to **1024*786** or **1280*1024**. If it is not, correct these settings (see chapter 3.4).

If your PC controls a spectrometer:

1. Click **Start → All Programs**

and check if you see the entry NFS Maestro. If it does not appear, install NFS Maestro Server as described in chapter 10.4.

2. Click **Start → All Programs → Accessories → Command Prompt**

enter: **ipconfig /all**

and check if the second Ethernet adapter is configured. If it is not, configure it as described in chapter 5.

11.1.1 The NMR SuperUser

During the installation of the NMR-SUITE, you will be prompted for the NMR SuperUser. In XWIN-NMR, the NMR SuperUser password is requested by certain commands like **cf**, **expinstall** etc. The NMR SuperUser can be Administrator (this is the default) or any other user. The NMR SuperUser can also be a Domain account. If you choose an NMR SuperUser other than Administrator make sure that this user exists under Windows XP (see chapter 14.1). For a local account the installation program will warn you if the specified account does not exist, but not for a Domain account. We recommend to install a special user for this purpose, e.g. a user named *nmrsu*. This user does not need any special permissions under Windows XP; standard access permissions are sufficient.

11.1.1.1 How to change the nmrsu after installation of NMR-SUITE

1. Double click on the icon 'Bruker Utilities' on the desktop

A window Bruker Utilities will appear

2. Double click on the command prompt

Note: It is not possible to use a 'normal' windows command prompt, because in

this 'special' command prompt of 'Bruker Utilities' there are several parameters and path entries defined.

3. Type in:

```
perl\bin\perl prog\bin\installnmr <XWINNMRHOME> <NAMEofNMRSU>
```

If you installed NMR-SUITE in the default directory and you like to use the user Administrator as NMR-SuperUser, you have to type in

```
perl\bin\perl prog\bin\installnmr C:\Bruker\XWIN-NMR Administrator
```

Note: You can use this command also for recreating the default permissions of installed Bruker files and directories

11.1.2 Converting a FAT filesystem to NTFS

The NMR-SUITE can only be installed on a NTFS filesystem, not on a FAT file system. However, you can convert FAT to NTFS as described in chapter 4.1.2.

11.2 Packages on the NMR Suite CDROM

1. XWIN-NMR: Acquisition and processing software
2. XWIN-PLOT: Object oriented WYSIWYG plot editor
3. ICON-NMR: Icon-driven interface for Routine Spectroscopy and Automation
4. NMR-GUIDE: Web-browser based teaching and training program
5. DISKLESS: Spectrometer CCU operating system
6. NMR-CHECK: Program for local spectrometer checks or remote service
7. NMR-SIM: Program for numerical simulation of NMR experiments
8. MAXENT: 1D/2D/3D spectrum deconvolution (requires separate license)
9. AMIX-Viewer: new multiple object viewer (requires a separate license)
10. AURELIA: Analysis of 2D/3D/4D NMR data (requires separate license)
11. AMIX: Analysis of Mixtures (requires a separate license)
12. GLP: Program for 'Good Laboratory Practice' tests (requires separate license)
13. FLEXLM: License manager required for starting NMR-SUITE programs.
14. GNU TOOLS: System tools required by XWIN-NMR.
(automatically installed as part of the XWIN-NMR package)

15. PERL: language interpreter required for certain XWIN-NMR commands.
(automatically installed as part of the XWIN-NMR package)

11.3 Installing the NMR Suite

This chapter describes the installation of the NMR-SUITE as local Administrator, using a local NMR SuperUser account. Chapter 5.6 describes additional steps which must be taken if you want to install the NMR-SUITE in a Domain. The installation program stores several log files in the directory \TEMP on the partition where Windows XP is installed, e.g. C : \TEMP.

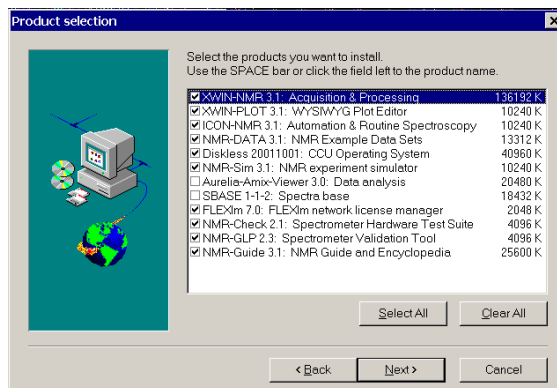
If NMR-SUITE 2.5 is already installed, and you want to re-install certain packages, first remove these packages according to chapter 2.3 and reboot the computer. If you want to upgrade from NMR-SUITE 2.6 to NMR-SUITE 3.x you can immediately start to install, the Installation Manager will automatically de-install the necessary programs. You could confirm the usual questions and have to log in after the reboot, the installation will then continue with the software products you have already selected.

!

1. Log in as Administrator
2. Close ALL WINDOWS on the desktop
3. If any X Server other than Exceed is running, stop it in the following way:
 - a) Press **CTRL+SHIFT+ESC** to start the Task Manager
 - b) Click **Applications**
 - c) Check if any *X Server* programs are running
 - d) For each running *X Server*: select it and click **End Task**
 - e) Close the '*Task Manager*' window by clicking the **X** button
4. Insert the CDROM '*NMR-SUITE for Windows 2000 / Windows XP*' Make sure you have the Windows XP version of it, and not the UNIX version. They look alike and a standard delivery contains both!
5. The windows '*Bruker NMR-SUITE Installation*' and '*Welcome to the Bruker Software Installation Manager*' will appear ¹:
→ Click **Next**

1. If this window does not appear Autorun is probably switched off (see chapter 2.4)

6. A window 'NMR-SUITE *Release Letter*' will appear:
 - a) Click **Yes** to read the NMR Release letter.
 - b) Please read the NMR Release letter!
 - c) Close the Release Letter by clicking the **X** button in the upper right corner.
7. A window '*Product Selection*' will appear:



- a) Select the packages which you want to install (note that DISKLESS is only required if your PC controls a spectrometer or you would like to configure him like a spectrometer control PC (see chapter 13.1.2)).

Do one of the following:

 - Accept the default selection (sufficient for spectrometer control)
 - Select/De-select packages according to your preference
 - b) Click **Next**
8. If the DISKLESS was selected in step 7, a window '*Information*' will appear:



If the PC is not yet connected to a spectrometer or if the CCU is not booted¹ you can promptly

- click **OK**

If your PC is currently connected to a spectrometer and the CCU is booted:

- a) Press the keys **CTRL+ESC** (to open the Start menu)
- b) Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- c) Enter: **rsh spect -l root /etc/init 5**
→ this will shut down the CCU
- d) Enter: **exit**
- e) Close the window *Information* by clicking **OK**

Note: The CCU is now either down or switched off and should be turned on again at the end of this procedure.

9. A window 'Select Installation Type' will appear:

- Click **Typical** (to install all packages in their standard directories.)²

10. If DISKLESS was selected in step 7 and if this package is already installed (any version) it is automatically deleted and a window 'Reboot' will appear:

- a) Click **OK** to reboot the computer
- b) Login as Administrator
- c) Eject and insert the CDROM to continue the installation

1. Note that during a first time installation of the NMR-SUITE the CCU can not be booted.

2. **Custom** installation is not described in this manual. It allows the user to determine in which directory each package will be installed; this is normally only necessary for installations of two different XWIN-NMR versions.

11. A window '*Set NMR Super User*' will appear ¹:

a) Do one of the following:

- Accept the default NMR SuperUser (Administrator) or
- Enter a special user for this purpose, e.g. named *nmrsu* or
- Enter any other user

If you choose an NMR SuperUser other than Administrator, and this user does not exist yet:

- Press the keys **CTRL+ESC** (to open the Start menu)
- Install a user as described in chapter 5.6.1.

b) Click **Next**

→ The installation of NMR-SUITE will start now.



12. It is strictly recommended to accept the default path for the flexLM installation: 'C:\flexlm' ! If you choose an user defined path you have to create a system variable to define the installation path as LM_LICENCES_FILE. This may cause some problems with other applications using the FlexLM.

13. If you selected NMR-SIM, AURELIA and/or SBASE for installation, several dialog windows will appear. Follow the prompts until you reach step 14.

14. A window '*Setup is complete*' will appear:

- You will be asked if you want to restart the computer:

a) Click **Yes I want to restart my computer now**

b) Click **Finish** (to reboot the computer)

15. After the PC has booted up, press the reset button on the CCU or turn it on with the key if it was switched off.

11.4 Installing NMR Suite patches

Bruker BioSpin recommends to install the latest NMR-SUITE patches available. First check the current patchlevel on your system by clicking on the icon **Bruker Utilities** on the desktop. Then click **Miscellaneous** → **Patchlevel** and the current patchlevel will appear. Now check if the Patchlevel on the Bruker BioSpin web server is higher than on your system:

1. Certain commands like *cf* and *expinstall* ask for the NMR SuperUser password.

<http://www.bruker-biospin.de/NMR/nmrsoftw/passwd/updates/pc/index.html>

All patches are contained in one self-extracting file with the extension .exe

Just copy this file to your PC and then click its icon. An install shield will appear, follow the instructions to install the patches.



Never remove the **XWIN-NMR** patches

If you start Add/Remove Programs from the Control Panel, the NMR-SUITE patches will appear as a separate package. However, separate removal of the patches is currently not supported. If you remove the patches, XWIN-NMR will not start any more and you will have to remove and re-install XWIN-NMR.

11.5 Installing a PDF Viewer

A PDF viewer is required for displaying the XWIN-NMR Online Help. A PDF viewer is not installed automatically as a part of XWIN-NMR. Bruker BioSpin recommends to use the Adobe Acrobat Reader. The Acrobat Reader is available from Adobe as a download:

<http://www.adobe.com>

11.6 Configuring the automatic start of the X-server

In some special situations it is necessary to define manually the path where the X-server is located. This configuration is only necessary if XWIN-NMR can not start because it does not find the X-server although there is a valid X-server available. For a detailed description of the installation and configuration of the X-server Exceed please refer to chapter 10.



- Click **Start** → **Control Panel** → **MKS Toolkit**
- In the upcoming window click on the field **NutC4 Options**
- In the field **Category** select **X Windows system settings**
- In the field **X Server settings** click on **other** and browse for the path of exceed.exe, default path is:

C:\Program Files\Hummingbird\Connectivity\7.11\Exceed\exceed.exe

- Click **OK**

11.7 Configuring NFS Server



If your PC is controlling a spectrometer, you must configure NFS after the installation of the DISKLESS package (part of the NMR-SUITE). This configuration requires that Hummingbird NFS Server is installed (see chapter 10.4). Once this is installed, you can mount any Windows directory from any UNIX host in your network (see chapter 5.4.4). Basically this chapter finishes the installation you started in chapter 10.4

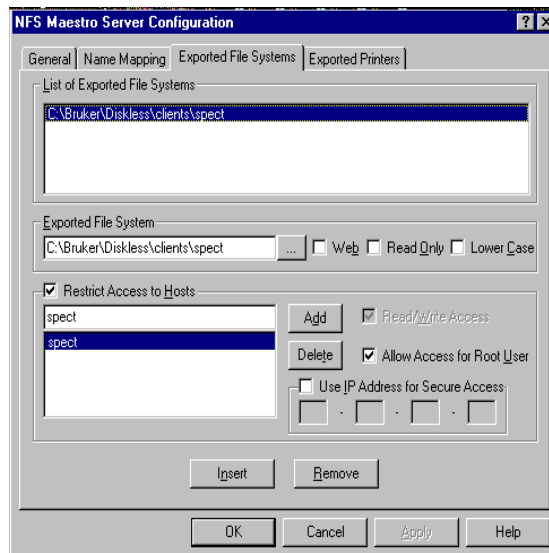
For this configuration it is very important to turn the Simple File Sharing off:

1. Double-click **My Computer** on the desktop.
 2. Click on **Tools**, select **Folder Options**.
 3. Click the **View** tab, and then click to select the **Use Simple File Sharing (recommended)** check box to enable Simple File Sharing (click to clear this check box to disable this feature).
1. Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
 2. Select the directory <XWINNMRHOME>\Diskless and click with right mouse button.
 3. Select in the upcoming window the entry **Properties**
 4. Choose the folder **Security**
 5. You should see **Full Control** permissions for **Everyone**. Correct this if necessary in the following way:
 - Click **Add**
 - A window *Select Users, Computers, or Groups* will pop up
 - choose the entry **Everyone** in the list **Names**
 - Click **Add**
 - Click **OK**
 - Enable in the 'Permissions' column 'Allow' **Full Control**
 - Click **OK**
 - In most cases especially if your PC controls a spectrometer some error messages could appear. A question if you really want do change the permissions in all the subdirectories of *Diskless* may also occur. You can click **OK** in all these windows

11.7.1 Configuring NFS Server 7.1

If you have NFS Server 7.1, proceed as follows:

1. Create the user
 - **'diskless_user_sys'** (with *'account is disabled'*)¹
 and the groups (with no members)
 - **'diskless_group_root'**
 - **'diskless_group_other'**
 - **'diskless_group_sys'**
2. Click **Start** → **Control Panel**
3. The window *'Control Panel'* will appear:
 - Double-click the icon **Hummingbird NFS Server**
4. A window *'NFS Maestro Server'* will appear:
 - a) Click the **Exported File Systems** tab



1. Creation and configuration of the necessary user and groups are most convenient if it is done in the user management tool of the management console and not in the user management of the control panel. For starting the management console click right on *'My computer'* and choose *'manage'*. A new window appears where you can choose *'local users and groups'*

- In the field **Exported File System**: browse for the location of the DISK-LESS package. For a typical installation on partition C: this is:

C:\Bruker\Diskless\clients\spect

Important: the Uppercase letters in this path are necessary!

- Select the **Allow Access for Root User**
- Select **Restrict Access to Hosts** (if it is not selected), enter **spect** in the field below and click **Add** → the name spect will appear in the list below '*Restricted Access to Hosts*'
- Click **Insert** → the name spect will appear in the 'Lists of Exported File Systems'

b) Click the **Name Mapping** tab

- Click the arrow to the right of the field *Load NT Names from* and select the local hostname, e.g. \\MYHOST
- Click **Reload Names**
- Adding a User mapping
 - In the field *User Name* select the user **Administrator**
 - In the field below, that is called '*UID*' type in '**0**'
 - Click **Insert**
 - In the field *User Name* select **diskless_user_sys**.
 - In the field below, that is called '*UID*' type in '**2**'
 - Click **Insert**
- Adding a Group mapping
 - Select the Group Name using the arrow button in the field below it, type in the GID and click **Insert**
 - Map the group **diskless_group_root** as group with GID 0
 - Map the group **diskless_group_other** as group with GID 1
 - Map the group **diskless_group_sys** as group with GID 3

c) Click the **General** tab

- Click **Server Status**
- A window '*NFS Maestro Server Status*' will appear:
 - Click **Reload Exports**
 - Click **OK**

5. In the window '*NFS Maestro Server Configuration*' → Click **OK**

6. If a message about the owner and permissions of spect appears:

- Click **Yes**
- A window '*Permissions*' will appear:
 - Select User: '*Adminsitrator*' and enable Read, Write and Execute permissions for this user
 - Select Group: '*diskless_group_root*' and enable Read, Write and Execute permissions for this group
 - Be sure that also '*other*' has Read, Write and Execute permissions
 - Click **Recursive** → Click **OK**

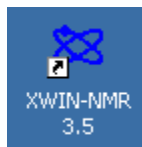
7. Close the window '*Control Panel*' by clicking the **X** button.

11.8 Adding a user to the group NmrUser

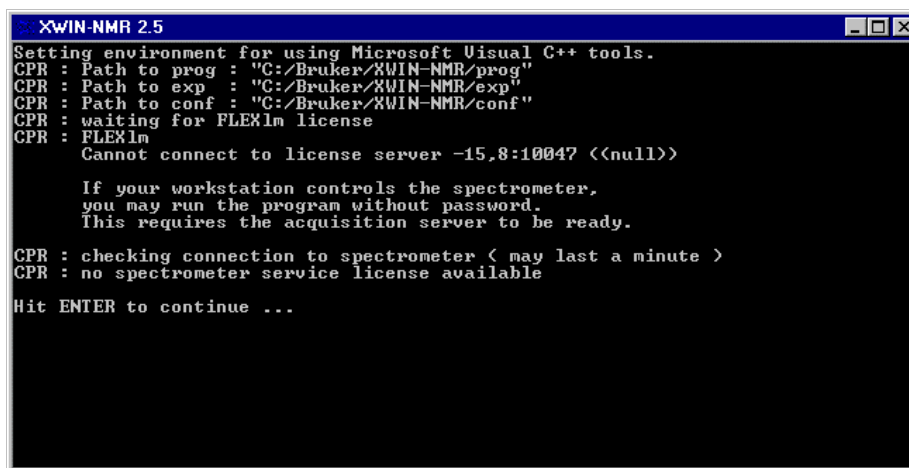
- ! Each user who wants to run XWIN-NMR must be member of the group NmrUser. Adding users to this group is described in chapter 14.1.3.

11.9 Check if the XWIN-NMR installation is correct

Double click the XWIN-NMR -icon



unless you already have a license you will get this screen:



```
XWIN-NMR 2.5
Setting environment for using Microsoft Visual C++ tools.
CPR : Path to prog : "C:/Bruker/XWIN-NMR/prog"
CPR : Path to exp  : "C:/Bruker/XWIN-NMR/exp"
CPR : Path to conf : "C:/Bruker/XWIN-NMR/conf"
CPR : waiting for FLEXlm license
CPR : FLEXlm
      Cannot connect to license server -15.8:10047 <(null)>

      If your workstation controls the spectrometer,
      you may run the program without password.
      This requires the acquisition server to be ready.

CPR : checking connection to spectrometer < may last a minute >
CPR : no spectrometer service license available

Hit ENTER to continue ...
```

11.10 Completing the NMR-GUIDE installation

There are two ways to start the NMR-GUIDE server (=gserver): manual and automatic.

If you often want to use the NMR-GUIDE remotely you should start it automatically so you can use its databases whenever someone is logged on the PC.

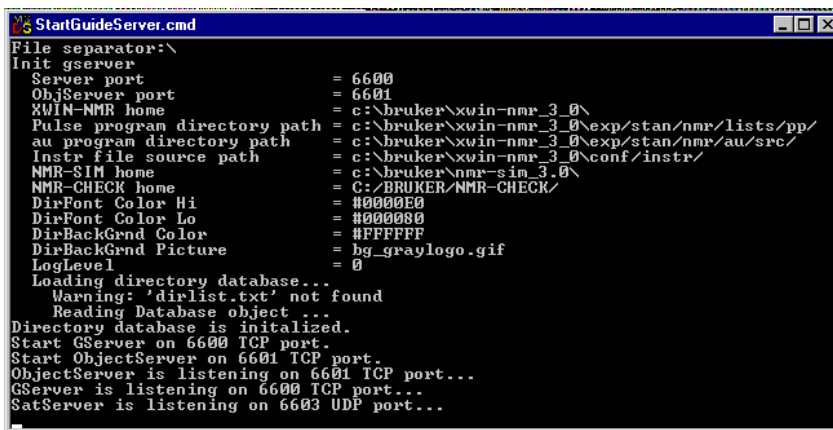
If you do not want to allow every user in your network to use the NMR-GUIDE whenever someone is logged on the PC, you should start it manual whenever you want to use the NMR-GUIDE.

Note: A PDF viewer is required for displaying documents (see chapter 11.5).

11.10.1 Manual starting of the NMR-GUIDE server

1. Double click the icon 'BRUKER Utilities' on your desktop
or click **Start** → **All Programs** → **Bruker NMR Suite** → **Bruker XWIN-NMR x.y** → **Bruker Utilities**
2. A window 'Bruker Utilities' appears
3. Double click *Miscellaneous*
4. Double click the entry *StartGuideServer.cmd* or *StartGuideServer*

5. A command prompt *StartGuideServer.cmd* will pop up



```

File separator:\
Init gserver
  Server port           = 6600
  ObjServer port        = 6601
  XWIN-NMR home         = c:\bruker\swin-nmr_3_0\
  Pulse program directory path = c:\bruker\swin-nmr_3_0\exp\stan/nmr/lists/pp/
  au program directory path  = c:\bruker\swin-nmr_3_0\exp\stan/nmr/au/src/
  Instr file source path     = c:\bruker\swin-nmr_3_0\conf\instr/
  NMR-SIM home            = c:\bruker\swin-nmr_3_0\
  NMR-CHECK home          = C:\BRUKER\NMR-CHECK/
  DirFont Color Hi        = #0000FF
  DirFont Color Lo        = #000080
  DirBackGrnd Color       = #FFFFFF
  DirBackGrnd Picture     = bg_graylogo.gif
  LogLevel                = 0
Loading directory database...
Warning: 'dirlist.txt' not found
Reading Database object...
Directory database is initialized.
Start GServer on 6600 TCP port.
Start ObjectServer on 6601 TCP port.
ObjectServer is listening on 6601 TCP port...
GServer is listening on 6600 TCP port...
SatServer is listening on 6603 UDP port...

```

6. Now open the Internet Explorer and type the URL

http://localhost/guide/test.html and *.../manual.html*

to check whether the test and/or the NMR-GUIDE are functional



*NOTE: It is convenient to copy the entry **StartGuideServer.cmd** onto your desktop. The next time you want to start the gserver just double click on this icon.*

11.10.2 Automatic start of the NMR-GUIDE

1. Log in as Administrator
2. Double click the icon **BRUKER Utilities** on your desktop
or click **Start → All Programs → Bruker NMR Suite → Bruker XWIN-NMR x.y → Bruker Utilities**
3. A window '*Bruker Utilities*' appears
4. Double click *Miscellaneous*
5. Click right on the entry *StartGuideServer.cmd* or *StartGuideServer*
6. In the context menu that appears, choose **create shortcut**
7. Click right on the entry *Shortcut to StartGuideServer.cmd* or *Shortcut to Start-GuideServer*
8. In the upcoming context menu choose **cut**
9. Click **Start → All Programs → Accessories → Windows Explorer**
10. Paste it into the directory:

C:\Document and Settings\All Users\Start Menu\Programs\Startup

11.10.3 Start the NMR-GUIDE on your spectrometer

1. Start XWIN-NMR
2. Type ***xau guide***

! *NOTE: Step 1. and 2. are only necessary if you want to use the NMR-GUIDE to control your spectrometer and to communicate with Xwin-nmr; e. g. for the graphical display of pulse programs*

3. Open the Internet Explorer
4. Open the page: *http://localhost/guide/manual.html*

11.10.4 Start the NMR-GUIDE remotely

1. Make sure that the gserver is running on the desired host (see chapter 11.10.1 and 11.10.2)
2. Open the Internet Explorer
3. Open the page: *http://<hostcomputer.domain>/guide/manual.html*

Chapter 12

The NMR Suite license

12.1 Questions and answers about the NMR Suite license

1. Which programs need a license?

XWIN-NMR, XWIN-PLOT, NMR-SIM, NMR-GUIDE and NMR-CHECK need a license. However, if you order a license for XWIN-NMR, you automatically get a license for all five programs. Note, that the NMR-CHECK license allows you to use the program for local hardware checks but this does not include remote service time from Bruker BioSpin.

If you do not have a license for XWIN-NMR, it will start up in an emergency mode if your PC is connected to a spectrometer. Also, one XWIN-PLOT session (without portfolio editor) can be started from within XWIN-NMR. However, NMR-SIM, NMR-GUIDE and NMR-CHECK will not run without a valid license.

ICON-NMR is always used in connection with XWIN-NMR and does not need an individual license.

AURELIA, AMIX, MAXENT, GLP and PARAVISION do need a license which must be ordered for each program separately.

2. Which license types are available and what are there contents?

There are four different license types. Their contents, restrictions and run of validity are listed in the following table. For more information please refer to the

Bruker license order form in the help menu of XWIN-NMR or on the web server:

<http://www.bruker-biospin.de/NMR/nmr-softw/passwd/docu/index.html>

or contact your local Bruker BioSpin representative.

license type	contents
Full	XWIN-NMR, XWIN-PLOT, NMR-SIM, NMR-GUIDE, NMR-CHECK
	run of validity: 15 years
	no restrictions
Demo	XWIN-NMR, XWIN-PLOT, NMR-SIM, NMR-GUIDE, NMR-CHECK
	run of validity: 3 months
	node locked, count 1, free of charge
Processing-Only (Linux only)	XWIN-NMR, XWIN-PLOT
	run of validity: 15 years
	processing-only
Teaching	XWIN-NMR, NMR-SIM
	run of validity: 15 years
	Node locked, count 1. XWIN-NMR can process only datasets which are older than 4 weeks or datasets created by NMR-SIM. One XWIN-PLOT session (without portfolio editor) can be started from within XWIN-NMR.

3. What kind of licenses do I need?

If you want to use XWIN-NMR 3.x you need a FEATURE line 'XWINNMR3' in your `license.dat` file. If you have 'XWINNMR' or 'XWINNMR2' you can only start XWIN-NMR 1.x resp. 2.x

If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously.

4. Which licensing program is used for the NMR-SUITE?

The Flexlm license manager is used and is delivered on the NMR-SUITE CDROM. The Flexlm package occupies about 3 MByte of disk space. It contains the '*lmgr*' license manager, the '*lmutil*' program, Help files and example `license.dat` file.

5. What are the requirements for the Flexlm to function:

- your PC must have an Ethernet card
- the network (TCP/IP) must be installed
- the network Service '*NetBIOS Interface*' must be installed

6. What is a *Floating* license?

Floating licenses are licenses that are available for more than one computer in a network. *Floating* licenses are issued based on the Host-ID of one particular computer. This computer becomes the "license server". All computers that can communicate with this "license server" computer can use the licenses managed by this computer. For this to work, the same license file must be installed on all participating computers, including the "license server". The Flexlm license manager software must only run on the "license server" computer.

A *Floating* license can have just one license for a program like Xwin-nmr. In such a case, the respective program can be started once on one computer in the network. If more than one license is available, as many copies of the program as are covered by the license can be started simultaneously. For example, if you have a license file with 5 licenses for Xwin-nmr, Xwin-nmr can be started 5 times from any 5 computers in the network.

The number of licenses is stated in the FEATURE for the respective program.

7. What is a *Node Locked* license?

A node-locked license allows you to start the respective program only on the computer with the Host-ID for which that license was generated. Typically, this license form is chosen for spectrometer computers. No other computer can use the license in the way described above for floating licenses.

8. I already have a *Floating* license on my SGI. Can I use it on a PC?

Yes, if the PC is connected to the SGI via Ethernet-TCP/IP. Just copy the file `license.dat` from the SGI to the PC:

```
from /usr/local/flexlm/Bruker/licenses/license.dat  
to c:\flexlm\Bruker\licenses\license.dat
```

9. If I have a *Floating* license for my PC, can I use it on a SGI?

Yes, if the PC is connected to the SGI via Ethernet-TCP/IP. Install the license on the PC and copy the file `license.dat` from the PC to the SGI:

```
from c:\flexlm\Bruker\licenses\license.dat
```

to `/usr/local/flexlm/Bruker/licenses/license.dat`

- 10.** I already have a *Node Locked* license on my SGI. Can I use it on a PC?

No, a *Node Locked* license can only be used on the host for which it was created.

- 11.** How do I know if my license is *Floating* or *Node Locked*?

You can recognize this from the syntax of the license FEATURES in the `license.dat` file:

on PC:

`c:\flexlm\bruker\licenses\license.dat`

on SGI/Linux:

`/usr/local/flexlm/Bruker/licenses/license.dat`

If the entry '*HOSTID=*' appears after the encrypted password, the license is Node locked and can only be used on the local PC

FEATURE XWINNMR3 bruker_ls 0.0 5-nov-2016 3 \

9B1EA0113CD53A883974 HOSTID=006008d244fe vendor_info=....

→ *Node locked* license for three parallel sessions of XWIN-NMR that can be started on the local PC

FEATURE XWINNMR3 bruker_ls 0.0 5-nov-2016 3 9B1EA0113CD53A883974 vendor_info=....

→ *Floating* license for three parallel sessions of XWIN-NMR that can be started on every PC in the local network

- 12.** How can I determine the hostid of my PC?

See chapter 12.2.2.

- 13.** How do I install a license (full or demo) on my PC?

See chapter 12.2.

- 14.** Does a Demo license require SERVER/DAEMON lines in `license.dat`?

No, a Demo license is *Node Locked* and therefore only requires FEATURE lines. If SERVER and/or DAEMON lines exist, they are ignored.

- 15.** I have a *Floating* license. Must the file `license.dat` be identical on all hosts, server and clients?

Yes, you can install `license.dat` on the server and then copy it to all clients.

- 16.** Must the Flexlm license manager run on all hosts in the network?

No, it only needs to run on the license server. If the license manager also runs on

a license client, this is simply ignored.

17. Must the Flexlm license manager run on a host with a Demo license?

No, it only needs to run on the server for *Floating* licenses.

18. What can I do if XWIN-NMR does not start after I installed the license?

See chapter 15 .

19. How is it possible that XWIN-NMR starts even though I do not have a license?

If you do not have a license for XWIN-NMR, it will start up in an emergency mode if your PC is connected to a spectrometer, Also one XWIN-PLOT session (without portfolio editor) can be started from within XWIN-NMR. However, NMR-SIM, NMR-GUIDE and NMR-CHECK will not run without a valid license.

12.2 Ordering and installing the NMR Suite license

12.2.1 Ordering a license

You can order a license by Fax or Email from Bruker BioSpin Germany. Demo licenses are free of charge, for other licenses you must specify your order number. Send a fax to +49 721 5161346 or an email to license@bruker.de, specifying:

- the hostid of your PC (see chapter 12.2.2)
- the program for which you want to get a license, e.g. XWIN-NMR
- the type of license, full, demo, processing-only or teaching
- the number of licenses and your order number (not necessary for demo license)

For a detailed description please refer to the license order form that is available on the Bruker BioSpin web server:

<http://www.bruker-biospin.de/NMR/nmrsoftw/passwd/docu/index.html>

12.2.2 How do I determine the correct hostid

The hostid is a 12-digit hexadecimal number. It is the physical address (also called Mac address or Node address) of the Ethernet card. After installing XWIN-NMR, including the Flexlm license manager, you can determine the hostid in two ways:

- Start XWIN-NMR; a command prompt will pop up, which will list the hostid, if a correct licence is not yet installed.

- Click the **Bruker Utilities** icon on the desktop, then click **Miscellaneous** → **get_hostid**
- Open a Command Prompt and type in:
`c:\flexlm\bruker\lmutil lmhostid`
 Under Windows XP it is possible to get more than one hostid. Just select one of them to order the license.

Some hostid values may indicate problems:

- If hostid '2' occurs: You may run Windows XP and your network-adapters are disabled.
 Click **Start** → **Control Panel** → **Network Connections**
 Right-click all **Local Area Connection xxx** -items and there click **Enable** (if it is visible)
- If hostid '0' or 'ffffff' occurs: You may run Windows XP and your network-adaptor has no link to the network.

Establish an link to the network or install the

NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:

Click **Start** → **Control Panel** → **Network Connections**

Right-click **Local Area Connection xxx**

Click **Properties** → **Install...** → **Protocol** → **Add**

The *Select Network Protocol*-menu will appear after some seconds.

Click **NWlink ...** → **OK**

After some seconds the Properties-menu will reappear: Click **Close**

See also

`C:\flexlm\Bruker\help\Index.htm`

for FlexLM-related problems

12.2.3 Installing a Demo license

A Demo license can be installed as follows:

1. Log in as Administrator
2. Install the Flexlm license manager as described in chapter 11.3.
3. Open a Command Prompt and enter:
 - `cd /d c:\flexlm\Bruker\licenses`

- **notepad license.dat**

enter the FEATURE lines, save and exit the file

Of course, you can also install the license file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (perhaps hidden) extension `.txt` to the file `license.dat` which makes it unusable (see chapter 16.1.3).

12.2.4 Installing a full license on a license server

The Flexlm license manager must always be installed and run as an Windows XP service on the license server. It is delivered on the NMR-SUITE CDROM and can be installed as described in chapter 11.3. The Flexlm is automatically installed as a Windows XP Service which is then automatically started.

On the license server, the file `license.dat` must contain a **SERVER** line, a **DAEMON** line and **FEATURE** lines. An example would be:

```
SERVER tulip 0060080e830d 1700
DAEMON bruker_ls c:\flexlm\Bruker\bruker_ls.exe
FEATURE XWINNMR3 bruker_ls 0.000 18-mar-2014 3 9B5EE07110D9CF96D0D2 \
vendor_info=" for hostid(s) : 0060080e830d"
FEATURE XWINPLOT bruker_ls 0.000 18-mar-2014 3 6B0EF0110296AB8030FC \
vendor_info=" for hostid(s) : 0060080e830d"
FEATURE NMRSIM bruker_ls 0.000 18-mar-2014 3 4B3E307115AF211AD2C5 \
vendor_info=" for hostid(s) : 0060080e830d"
FEATURE NMRGUIDE bruker_ls 0.000 18-mar-2014 3 7C3FE1B212FGB8809EG2 \
vendor_info=" for hostid(s) : 0060080e830d"
FEATURE NMRCHECK bruker_ls 0.000 18-mar-2014 3 6B4ED0A101EFA7798DF1 \
vendor_info=" for hostid(s) : 0060080e830d"
```

where *tulip* is the hostname and *0060080e830d* the hostid of the computer. Note that the second part of the **FEATURE** lines, the `vendor_info`, does not necessarily exist. In that case a **FEATURE** line would look like:

```
FEATURE XWINNMR3 bruker_ls 0.000 18-mar-2014 3 9B5EE07110D9CF96D0D2 ""
```

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmttools.exe`
2. A window '**LMTOOLS**' appears. Click the **Start/Stop/Reread** tab → Click **Stop Server** → Click **Start Server** → Click **ReRead License file** → Click **OK**

3. Close the window '*LMTOOLS*' by clicking the **X** button.

12.2.5 Installing a full license on a license client

On a license client, license can be installed in two different ways, as described for a Demo license chapter 12.2.3. The only difference is that you do not have to setup a new file `license.dat`. You can just copy it from the license server which can be another PC or an SGI (see questions 8 and 9 in chapter 12.1).

12.2.6 Modifying the license file

To inform Flexlm about the new license proceed as follows:

1. Open the **Windows Explorer** and go to `<Flexlm_Home>\Bruker\` → Double-click `lmttools.exe`
2. A window '*LMTOOLS*' appears. Click the **Start/Stop/Reread** tab → Click **Stop Server** → Click **Start Server** → Click **ReRead License file** → Click **OK**
3. Close the window '*LMTOOLS*' by clicking the **X** button.

12.2.7 Further information

For more information on the Flexlm license manager:

Click **Start** → **run** enter `c:\flexlm\bruker\help\index.htm` click **OK**

If XWIN-NMR does not start after installing the license, please check chapter 15

Chapter 13

Configuration of XWIN-NMR

The idea of this chapter is to give you some guidelines to full spectrometer or workstation configuration. We do not discuss the commands in detail here. For a full description refer to the XWIN-NMR manual.

13.1 Configuring XWIN-NMR

There are two ways to start XWIN-NMR:

1. Click the icon XWIN-NMR on the desktop
2. Click

Start → All Programs → Bruker NMR Suite → XWIN-NMR<vers.>

After the first startup of XWIN-NMR you have to configure the software (depends on the hardware of your spectrometer). If you do this, you are mainly in one of the four following situations:

- You have just done a software update
so the old spectrometer configuration of the software is still known to the new version → go to chapter 13.1.1
- You want to configure a only-processing-PC like your spectrometer-PC
so you have the spectrometer configuration on another computer → go to

chapter 13.1.2

- You have to configure the software on a new hard disk without a backup of the spectrometer configuration
so you have no configuration files anymore → go to chapter 13.1.3
- You have a new spectrometer hardware component
so you have no configuration file so far → go to chapter 13.1.3

13.1.1 If your PC controls a spectrometer:

1. Be sure that the spectrometer is booted (see chapter 11.3 and 15.4.3)
2. Type **edc** and create a new dataset
 - Do not configure in the default dataset `'exam1d'` or `'dEfAuLt'`.
 - You can also select an already existing dataset acquired with another XWIN-NMR version
3. Enter **config**

A window *'configure'* will appear showing a list of configuration steps. Accept the default selection and click **Start**. You will be asked for the superuser password a couple of times:

- The command **cf** now configures the software according to the hardware of your spectrometer
 - a) *Configuration of <spectrometer-name>. Change that? (yes/no)*
Most likely you will type **no** → **ENTER**, because the spectrometer-hardware has not changed
 - b) *Which type of spectrometer? Avance AMX ARX ...*
Choose the type of your spectrometer e. g. **AVANCE** → **ENTER**
 - c) Only in some cases:
Which type of Avance?
Type in the kind of your Avance e. g. **DRX** → **ENTER**
 - d) *Basic 1H frequency ... in MHz*
Type in the 1H-frequency e. g. **500.13** → **ENTER**
 - e) The *RS232 Channel for external devices*-Table appears

Check if the tty-numbers of the hardware components are set correctly then click **Save**

- f) Only if you have a sample changer

Should the Sample Changer control the Lift? (yes/no)

The answer depends on how the air flow is connected, normally you will answer: **yes** → **ENTER**

In this cases the question appear:

Delay between SX and next command [sec]?

Type in the length of the delay e. g. **10** → **ENTER**

- g) The *nuclei-table* appear

Check if the frequency of the nuclei are set correctly. If in doubt click **Re-store** then click **Save**

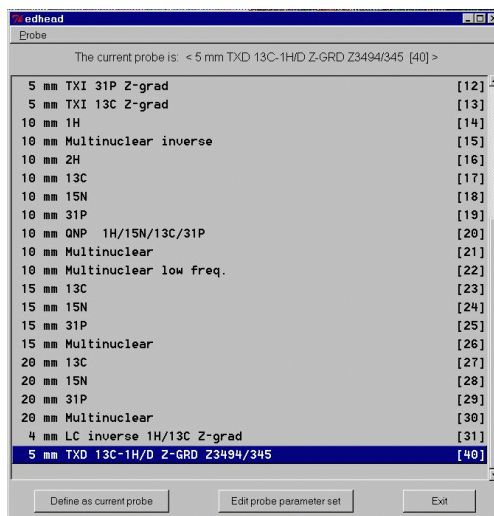
- h) The results of **cf** appears in a text window. Check this list carefully and compare the result with an list from an earlier configuration (if available) click **Print** and store the paper output with your other spectrometer documentation, then click **OK**



If during 'cf' an error message occurs that invites you to do a firmware update see chapter 13.3

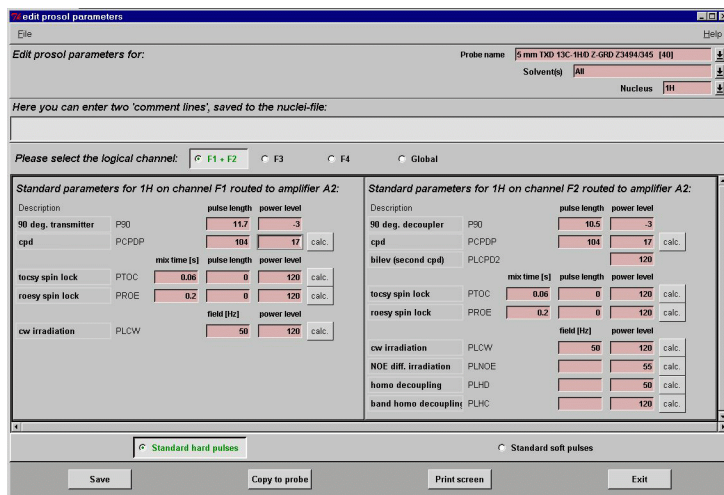
- Only if you have a temperature unit: **Continue** with **cfte**
check the tty of the temperature unit and press **enter** if it is correct
- **Continue** with **edsolv**
check the list of lock solvents and click **Save** if it is correct

- *continue with edhead*



select the current probe, click the button *Define as current probe* then click *Exit*

- *Continue with edprosol*



check the parameters for your favourite nuclei, change them and calculate them, if necessary, then click *Save* to store to disk

- *Continue with locnuc*

check the lock nucleus (most likely 2H), press **Enter** if correct

- *Continue* with **edlock**

check the lock table values (field, lock phase, ...), change them and click **Save** if necessary, otherwise click **Abort**

- *Continue* with **edscon**

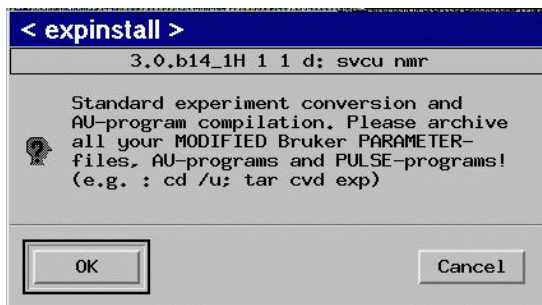
check the spectrometer constants, change it and click **Save** if necessary, otherwise click **Cancel**

- *Continue* with **edsp**

check the routing, change it and click **Save** if necessary, otherwise click **Cancel**

- *Continue* with **expinstall**

a) Click **OK** if you either have no modified Bruker BioSpin-Parameterfiles,



AU-programs and Pulse-programs or if you have archive them in a different directory. Your individual Parameterfiles, AU-programs and Pulse-programs that are named different from the original Bruker BioSpin files will not be destroyed during the installation

b) *Select Spectrometer Type*

Check if the highlighted system is yours, change if necessary then click **Proceed**

c) *Select Items for Installation-Table* appears

Click the functions you want to activate

(e. g. all except *Recompile All User AU Programs*)

d) *Select the type of digitizer*

There is usually only one option, but there could be choice. In that case, select the digitizer that you want to be used predominantly for automation

e) *Select acquisition mode*

Select the acquisition mode. Select *qsim* or *DQD* (if available). *DQD* gives the best baseline

f) *Enter default pre-scan-delay DE*

the default is 6 μ s, press **Enter** if you agree

g) *Select printer*

select the printer of your choice

h) *Select plotter*

select the plotter of your choice

i) *Enter paper format*

type in the paper format of your choice

and wait ...

After expinstall has finished insert a sample and make sure that you can lock on the lock solvent. If you have a temperature unit that **edte** starts without errors.

Type **ii** and read with **rpar** a standard proton parameter file, type **getprosol** and **rga** and collect a normal ^1H NMR spectrum.

13.1.2 If you want to configure a processing-PC like your spectrometer-PC:

If the PC does not control a spectrometer but is used in connection with a particular spectrometer, e.g. for setting up experiments, processing and or plotting, you should configure it as that spectrometer (see FAQ 210 on www.bruker-biospin.de): for example the spectrometer is a DRX400 configured with the name 'drx400'. The PC is called 'work1' and should be configured exactly like the DRX400. Do the following.

Note: It is necessary to install 'Diskless' from the Bruker BioSpin NMR-SUITE CD

- Copy the directory '<XWINNMRHOME>/conf/instr/drx400' from the spectrometer DRX400 to the workstation.
 - On the workstation, become superuser and paste this 'drx400' directory to '<XWINNMRHOME>/conf/instr'.
- (most likely this is the path: c:\Bruker\Xwin-nmr\conf\instr)
- Start XWIN-NMR as normal user.

- d) Type **edc** and create a new dataset
 - Do not configure in the default dataset '*exam1d*' or '*defAuLt*'.
 - You can also select an already existing dataset acquired with another XWIN-NMR version
- e) Run the 'cf' command:
 - *Configuration for <spect>. Change that? (y/n)* - Type in **y**
 - *Enter new instrument name* - Type in **station**
 - *Which type of spectrometer? Avance AMX ARX ASX Datastation* - Type in **Datastation**
 - *Basic 1H frequency (with offset O1=0) in MHz?* - Confirm the default '400.13' by pressing **Enter**
 - *Nuclei table for BSMS(b) or SCM(s) or ignore(i)?* - Type in **b**
- f) Save the table of basic frequencies which is displayed at the end of the **cf** dialogue
- g) Click on **OK** on the listed *Configuration Information*
- h) Open the file <XWINNMRHOME>/conf/instr/curinst as superuser. Modify its entry *station* to *drx400*, save and close the file.
- i) The procedure is now completed. Now run **expinstall** as if you would be on a spectrometer

13.1.3 If you do not know the configuration of your spectrometer



If you do not have any spectrometer configuration information, e. g. after a head-crash, then you have to recreate the configuration information.

In this situation there are two possibilities:

- a) your spectrometer has a standard configuration
- b) your spectrometer has a non-standard configuration

Case a)

If your spectrometer has a standard configuration, then you can easily do **cf** and if you give the correct information for the '*Type of Spectrometer*' you will get the correct list of your hardware in the '*RS232 table*'. You only have to type in the correct tty's of the interfaces.

Case b)

If your spectrometer has a non-standard configuration, then the hardware configuration is read during the **cf** from the file 'hardware_list' file in the directory

```
<Xwin-nmr-Home>\conf\instr\<spectrometer-name>
```

Because this file does not exist you have to do the following:

- Enter **cf makelist** in the XWIN-NMR window
this will create a file 'hardware.exam' in the directory

```
<XWINNMRHOME>\conf\instr
```
- Open this file with a text editor, e. g. notepad, and delete all lines except those that describe the hardware components of your spectrometer. You can get this information in the following way:

check the list in the file 'hardware.exam' with the components of your spectrometer and/or with the Bruker BioSpin delivery note(s). Please carefully check the PN-C/D/E and ECL numbers of the components

- **Save** and **exit** from 'hardware.exam'
- Copy the modified file 'hardware.exam' into the directory

```
<XWINNMRHOME>\conf\instr\<spectrometer-name>
```
- Rename the file

```
<XWINNMRHOME>\conf\instr\hardware.exam to  
<XWINNMRHOME>\conf\instr\hardware_list
```

13.1.4 If you added a new hardware component to your spectrometer



If you want to add a new hardware component it is recommended to order somebody of your local Bruker BioSpin office to do this for you.

If you have to add a new hardware component to the configuration file of the software, do the following:

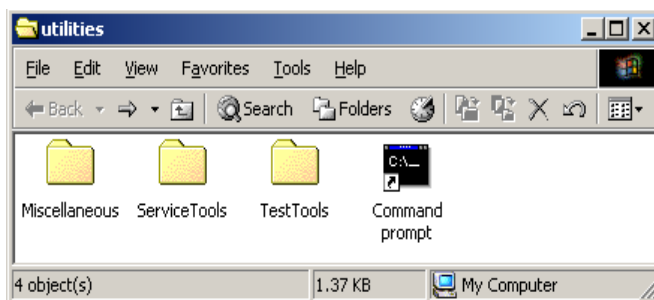
- Enter **cf makelist** in the XWIN-NMR window
this will create a file 'hardware.exam' in the directory

```
<XWINNMRHOME>\conf\instr
```


- Open this file with a text editor, e. g. notepad, and search and copy these line(s) that describe the new hardware component(s). Please carefully check the PN-C/D/E and ECL number(s) of the component(s).
- Copy the file
`<XWINNMRHOME>\conf\instr\spect\hardware_list` to
`<XWINNMRHOME>\conf\instr\spect\hardware_list_sav`
- Open the file
`<XWINNMRHOME>\conf\instr\spect\hardware_list`
and paste the new entries to the correct positions.

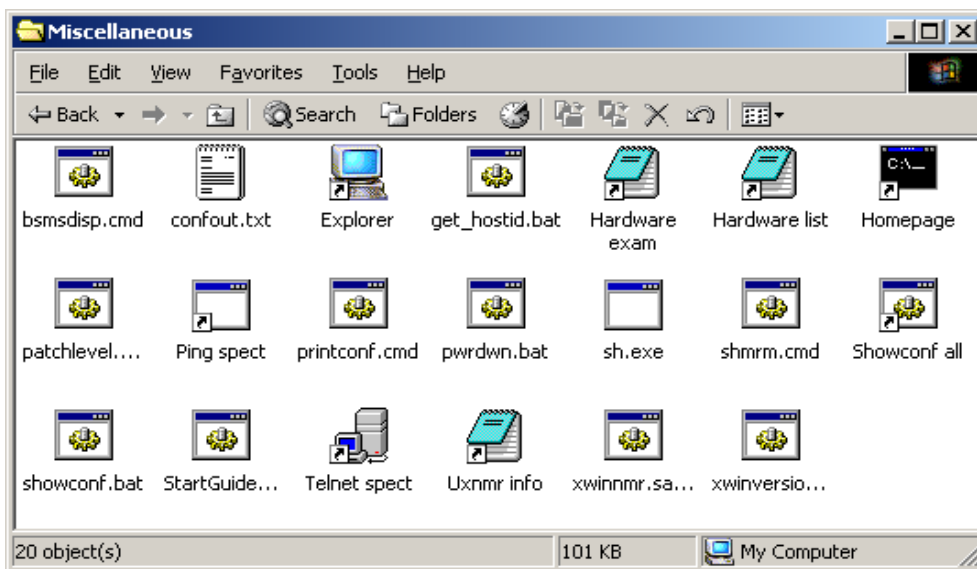
13.2 How to use the Bruker Utilities Folder

After a successful installation of the NMR-SUITE, you will find a new folder on every user's desktop named 'Bruker Utilities'. Double click on the folder to see its contents:

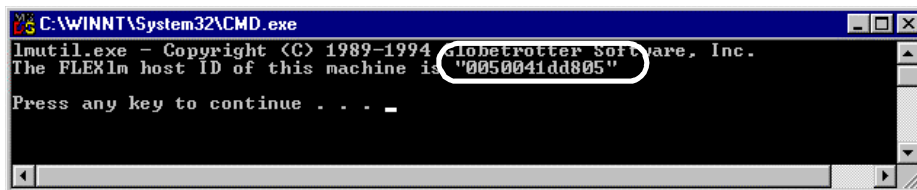


In this Utilities folder, you will find commands and applications that you might need when running and configuring a spectrometer. You can see the command prompt right there: just double click on it to get to the prompt.

The other tools are stored in three categories as shown above. You can double click on each of the folders to have them opened up to show their treasures:



Each of them (our example here is 'miscellaneous') have a number of batches or executables, or plain commands that you can run by just double clicking on the respective icon. For example, to see the system ID of the current PC you can just double-click on the icon called 'get_hostid' (highlighted in the screen shot above). It will open a text window and deliver the system ID you need to know when you apply for XWIN-NMR license (encircled):



If you press any key, the window will be closed again.

As you can see from the next screen (produced by the command `ipconfig /all` in a command prompt) flexlm takes the address of one of the Ethernet cards in the PC. Which one is used depends on the binding order of the two cards. You can check the binding by clicking the Network icon from the Control Panel.

```

C:\>ipconfig /all

Windows NT IP Configuration

    Host Name . . . . . : hh029498.brucker.com
    DNS Servers . . . . . : 10.1.32.2
                           10.1.32.1
    Node Type . . . . . : Broadcast
    NetBIOS Scope ID. . . . . :
    IP Routing Enabled. . . . . : No
    WINS Proxy Enabled. . . . . : No
    NetBIOS Resolution Uses DNS : No

Ethernet adapter E190x2:

    Description . . . . . : 3Com 3C90x Ethernet Adapter
    Physical Address. . . . . : 00-50-04-05-72-10
    DHCP Enabled. . . . . : No
    IP Address. . . . . : 149.236.99.1
    Subnet Mask . . . . . : 255.255.255.0
    Default Gateway . . . . . :

Ethernet adapter E190x1:

    Description . . . . . : 3Com 3C90x Ethernet Adapter
    Physical Address. . . . . : 00-50-04-1D-D8-05
    DHCP Enabled. . . . . : No
    IP Address. . . . . : 10.1.222.1
    Subnet Mask . . . . . : 255.255.0.0
    Default Gateway . . . . . : 10.1.32.3

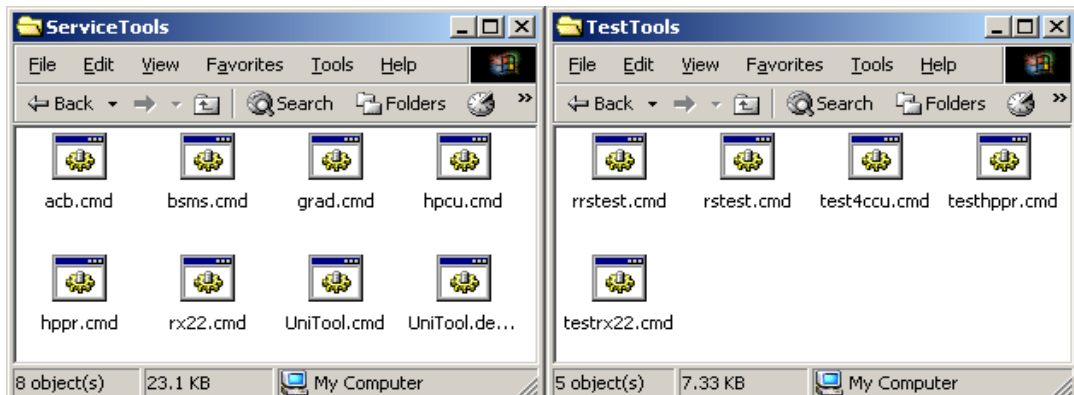
C:\>

```

Another interesting tool in the 'miscellaneous' section actually issues commands to the CCU rather than to the PC:

One of the items is 'pwrdown' in this category that logs in to CCU and issues the UNIX command that powers down the CCU. All YOU do is double click on it and watch it do the rest.

The other categories are 'Test Tools' and 'Service Tools':



You can just double-click the appropriate icon and the command-shell and tool programs will start up automatically.

13.3 Firmware update of the spectrometer hardware

This chapter describes how to update the firmware of certain spectrometer components. This is only necessary if the cf command has crashed and popped up a message window which informs that you have to do a firmware update of a component.



It is strongly recommended to do the firmware update only in this case, because the hardware component could get unusable if the update would be done incorrectly.

Start the '*Service Tools*' of the '*Bruker Utilities*' to check the firmware version of your spectrometer hardware. Double click on an icon starts an automatic procedure that will pop up a command prompt. The following example shows the check of the '*bsms-service tool*'

```

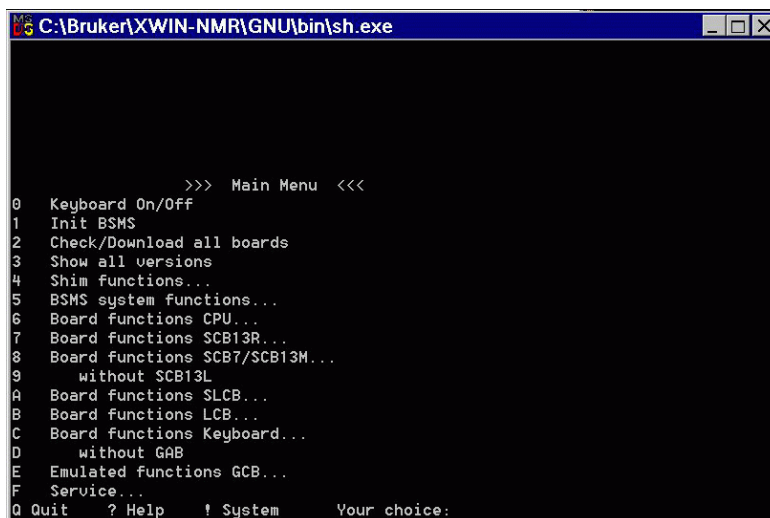
C:\Bruker\XWIN-NMR\GNU\bin\sh.exe

XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XX                                                                    XX
XX          ! ! !   W A R N I N G   ! ! !                             XX
XX                                                                    XX
XX          This is a hardware level debug tool.                      XX
XX          Improper operation may damage your hardware.                XX
XX                                                                    XX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
*          >>> bsms service toolbox <<<                               *
*                                                                    *
*          Version:      bsms      2.7                                *
*          Compilationdate: 000519                                     *
*          Author:       R.Eggli, M.Schenkel, R.Sauter                 *
*                                                                    *
*          Copyright (c) 2000 by Bruker AG, Faellanden Switzerland     *
XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX
Press Return to abort or 'y' to continue:

```

type **y** → **ENTER**

a dialog comes up in the command prompt



```

C:\Bruker\XWIN-NMR\GNU\bin\sh.exe

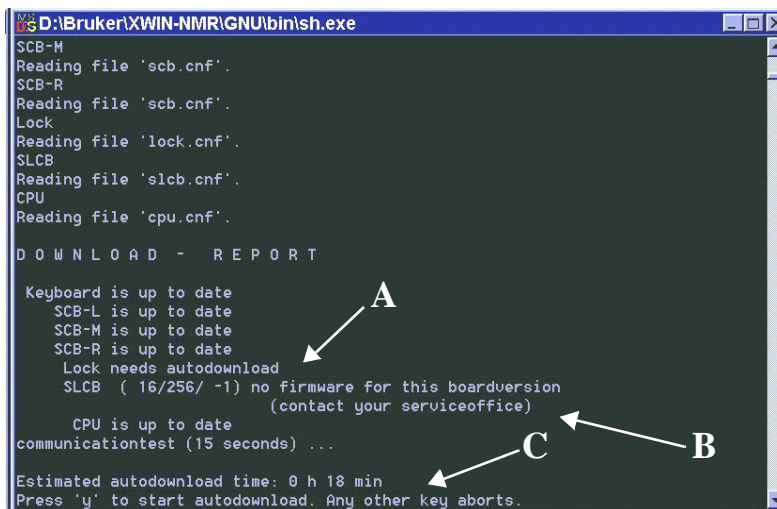
>>> Main Menu <<<
0 Keyboard On/Off
1 Init BSMS
2 Check/Download all boards
3 Show all versions
4 Shim functions...
5 BSMS system functions...
6 Board functions CPU...
7 Board functions SCB13R...
8 Board functions SCB7/SCB13M...
9   without SCB13L
A Board functions SLCB...
B Board functions LCB...
C Board functions Keyboard...
D   without GAB
E Emulated functions GCB...
F Service...
Q Quit   ? Help   ! System   Your choice:

```

To check and eventually download a new firmware (from XWIN-NMR) type

2→ENTER

The check starts and ends for example as shown in the following picture



```

D:\Bruker\XWIN-NMR\GNU\bin\sh.exe

SCB-M
Reading file 'scb.cnf'.
SCB-R
Reading file 'scb.cnf'.
Lock
Reading file 'lock.cnf'.
SLCB
Reading file 'slcb.cnf'.
CPU
Reading file 'cpu.cnf'.

D O W N L O A D   -   R E P O R T

Keyboard is up to date
SCB-L is up to date
SCB-M is up to date
SCB-R is up to date
Lock needs autodownload
SLCB ( 16/256/ -1) no firmware for this boardversion
(contact your serviceoffice)

CPU is up to date
communicationtest (15 seconds) ...

Estimated autodownload time: 0 h 18 min
Press 'y' to start autodownload. Any other key aborts.

```

Diagram labels in the image:

- A** points to "Lock needs autodownload"
- B** points to "(contact your serviceoffice)"
- C** points to "Estimated autodownload time: 0 h 18 min"

- if there is a problem with a component you get an information to contact your serviceoffice (B)

- if you need a firmware update you will get a message (A) with the length of time for the download (C). It is recommended to do the download as soon as possible.



During the download it is absolutely necessary that spectrometer and PC are not disturbed! Make sure that no one pull out a cable out of the spectrometer or will crash Windows XP while using it parallel! (Yes we know this seems very improbable, but if the download would crash your board might be unusable afterwards)

press **y** → **ENTER** to start the download

```
D:\Bruker\XWIN-NMR\GNU\bin\ish.exe

Keyboard is up to date
SCB-L is up to date
SCB-M is up to date
SCB-R is up to date
Lock needs autodownload
SLCB ( 16/256/ -1) no firmware for this boardversion
(contact your serviceoffice)
CPU is up to date
communicationtest (15 seconds) ...

Estimated autodownload time: 0 h 18 min
Press 'y' to start autodownload. Any other key aborts. y

Lock ( 16/ 8/ 0) autodownload with firmware (lockah.hex)
Reading file 'lockah.hex'.
check HEX-file (Intel) ...
Erasing FLASH memory...

Programming record: 3050 of 4940
Communication error detected and fixed

ERROR: 0201 No such file or directory

Press RETURN to continue...
```

A normal error during downloading the new firmware (see above) requires to do the download once again!

If you have done a download of newer firmware, you have to do **cf** again!

If you do not need any downloads you can follow the instructions in the command prompt to end this tool.

13.4 Configuring the BSMS-Keyboard

For a full description how to configure the BSMS-Keyboard see your

- hard copy of '*BSMS-User Manual*' or

- the respective entry on the '*BASH*' CD-ROM' (Order Number Z36541)

A configuring step that should be done periodically is the spin rate calibration. For this you have to go into the **Menu** mode of your BSMS keyboard:

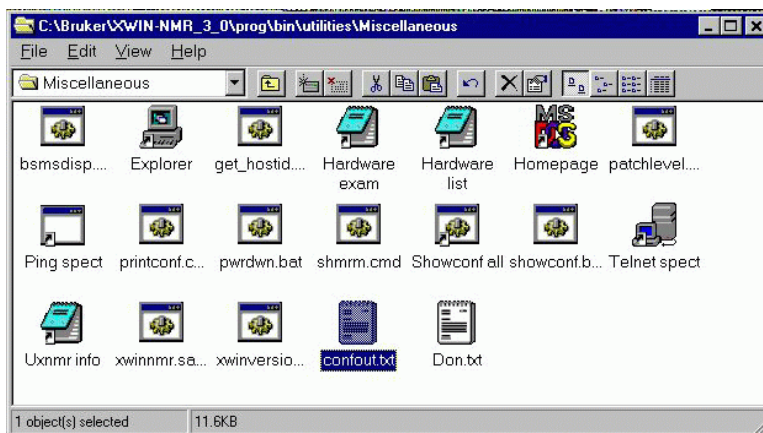
press simultaneously **2nd** and **Y³**, then rotate the control knob as long as you see **1.Sample** in the display, press **2nd** to go into this directory. The display will show **1.1 Spin calib.** press **2nd** to start this process and wait for ~ 3 minutes.

In this Menu mode, you can also define the helium warning level. If the liquid helium reaches the critical point, the BSMS-Keyboard starts beeping. A special password, the so called security code, is required to be able to change the setting. If in doubt about the setting, contact your service representative.

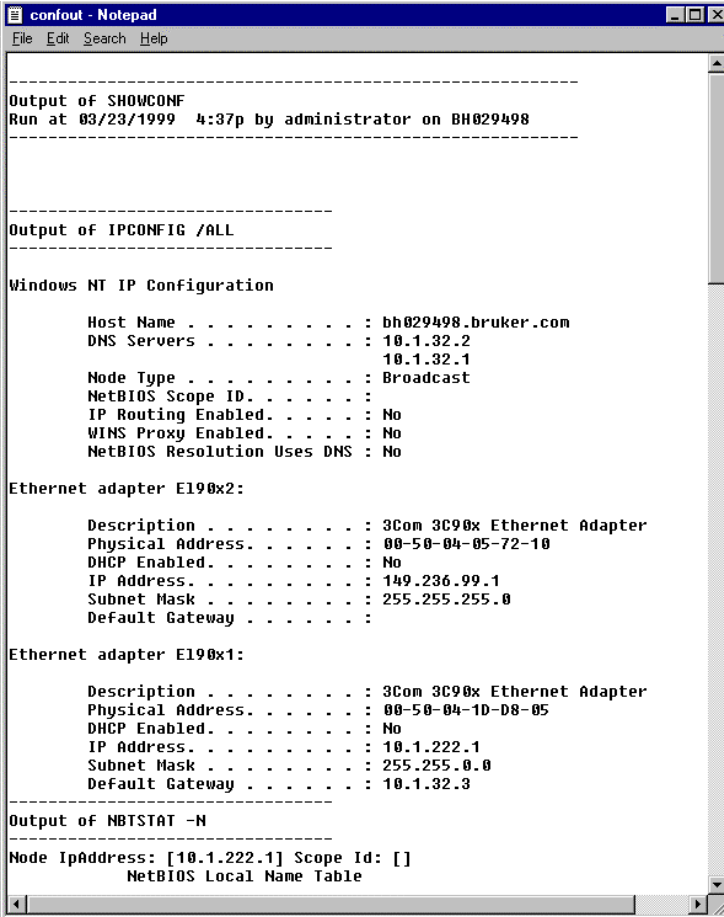
For an additional possibility to get a warning about a low helium level see chapter 21.4.

13.5 A log of the entire system configuration

The '*showconf*' command provides you with various information about your hardware and software, both of the PC and of the spectrometer. Here is how showconf works: You double-click on the respective icon in the folder **Miscellaneous** in the **Bruker Utilities** - and wait the about 2 minutes until it has finished. After that showconf has produced a file called `confout.txt` that contains all you need. `Confout.txt` is located next to the showconf batch after the first execution and you edit it from there:



Just double click on the confout icon to call the appropriate editor:



```

confout - Notepad
File Edit Search Help

-----
Output of SHOWCONF
Run at 03/23/1999  4:37p by administrator on BH029498
-----

-----
Output of IPCONFIG /ALL
-----

Windows NT IP Configuration

        Host Name . . . . . : bh029498.brucker.com
        DNS Servers . . . . . : 10.1.32.2
                                10.1.32.1
        Node Type . . . . . : Broadcast
        NetBIOS Scope ID. . . . . :
        IP Routing Enabled. . . . . : No
        WINS Proxy Enabled. . . . . : No
        NetBIOS Resolution Uses DNS : No

Ethernet adapter E190x2:

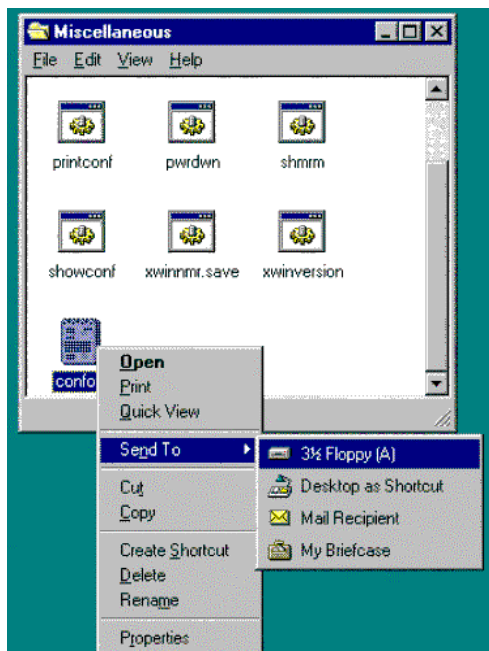
        Description . . . . . : 3Com 3C90x Ethernet Adapter
        Physical Address. . . . . : 00-50-04-05-72-10
        DHCP Enabled. . . . . : No
        IP Address. . . . . : 149.236.99.1
        Subnet Mask . . . . . : 255.255.255.0
        Default Gateway . . . . . :

Ethernet adapter E190x1:

        Description . . . . . : 3Com 3C90x Ethernet Adapter
        Physical Address. . . . . : 00-50-04-1D-D8-05
        DHCP Enabled. . . . . : No
        IP Address. . . . . : 10.1.222.1
        Subnet Mask . . . . . : 255.255.0.0
        Default Gateway . . . . . : 10.1.32.3

-----
Output of NBTSTAT -N
-----
Node IpAddress: [10.1.222.1] Scope Id: []
        NetBIOS Local Name Table
  
```

The easiest way to copy it on a diskette is right from within the miscellaneous-folder: Right-click on the confout-icon and select 'send to' and then A:



The size of this report is mostly less then 100 kbytes.

DO KEEP A COPY OF THIS FILE IN A SAFE PLACE!

13.6 Backup of VIF's (=Very Important Files)

It is not only necessary to create some backups for the operating system like ERD and Boot Disks and to store the acquired datasets,



it is strictly recommended to create a frequently backup of the 'VIF's' - the 'Very Important Files' of the configuration of XWIN-NMR.

There are many reasons like e. g. head crash or larceny of the hard disk that are requires to store weekly or monthly the important data in a way that you are able to restore the habitual spectrometer configuration in an appreciable short time.

XWIN-NMR 3.1 and higher offers a script for saving those important files that are not delivered by BRUKER. This script can save and extract user specific data from the <XWINNMRHOME> directory and puts them into a tar-file. Files that start with

an "." are ignored. The script can be started as follows:

Click on the Bruker Utilities icon on the desktop

Bruker Utilities* → *Miscellaneous* → *xwinnmr.save.cmd

For more information open the command prompt of the Bruker Utilities

Bruker Utilities* → *Command prompt and enter

`.\prog\bin\utilities\miscellaneous\xwinnmr.save -help`

Files and directories will be saved into the special tar-file `xwin_backup.tar` which is, by default, in the directory `<XWINNMRHOME>/xwin_backup`.

The following directories are saved completely (hidden files are ignored!):

`<XWINNMRHOME>/exp/stan/nmr/lists/group`

`<XWINNMRHOME>/exp/stan/nmr/lists/scm`

`<XWINNMRHOME>/exp/stan/nmr/lists/bsms`

`<XWINNMRHOME>/exp/stan/nmr/lists/mac`

`<XWINNMRHOME>/exp/stan/nmr/lists/fl`

`<XWINNMRHOME>/exp/stan/nmr/lists/ds`

`<XWINNMRHOME>/conf/instr/<spect>/prosol`

`<XWINNMRHOME>/conf/instr/<spect>/cortab`

`<spect>` represents the current spectrometer name or the name specified explicitly when ***xwinnmr.save*** is started.

From the following directories every file is saved that does not belong to the genuine Bruker distribution:

`<XWINNMRHOME>/exp/stan/nmr/lists/pp`

`<XWINNMRHOME>/exp/stan/nmr/lists/cpd`

`<XWINNMRHOME>/exp/stan/nmr/lists/gp`

`<XWINNMRHOME>/exp/stan/nmr/lists/wave`

`<XWINNMRHOME>/exp/stan/nmr/au/src`

`<XWINNMRHOME>/exp/stan/nmr/par`

<XWINNMRHOME>/plot/layouts

Additionally, the following files are also saved:

<XWINNMRHOME>/uxnmr.par

<XWINNMRHOME>/uxnmr.info

<XWINNMRHOME>/hardware_list

The options for **xwinnmr.save** [-options] are:

- **help** this message
- **path <x>** absolute path where backup tar-file xwin_backup.tar will be created
- **restore <x> <y>** absolute path where backup tar-file xwin_backup.tar can be found and absolute path where the restoring should take place (installation directory of XWIN-NMR)
- **replace** overwrite the old backup.tar file
- **silent** do not display any messages
- **spect <x>** spectrometer name (e.g. spect; default is the current name)
- **verbose** print more information while backing up

For safety reasons the tar-file will not be replaced by executing the **xwinnmr.save** script once again. So if you like to use the script several times, you have to move the xwin_backup.tar file from the directory <XWIN-NMRHOME>/xwin_backup on a backup medium (floppy, CD ...) and then start the script once again or you have to use the 'replace' option.

Chapter 14

User Management

14.1 User Management in a standalone PC

After the installation of Windows XP, there is one user with administrator rights, namely the user 'Administrator'. If the password for this user gets lost, there is no way of resetting it other than re-installing Windows XP. Therefore, we strongly recommend you install at least one more user with administrator rights, e.g. with the name 'root' (actually, this name is also much easier to type on the keyboard). You can install a new user or administrator as follows:

14.1.1 Adding a new user in a standalone PC (method 1)

The following chapter describes how to add a new user with Administrators rights:

1. Log in as Administrator
2. Click **Start** → **Control Panel** → **User Accounts**
3. A window '*UserAccounts*' will appear:
 - Click **Create a new account**
4. A window '*UserAccounts*' will appear
 - Enter the name of the new account e. g. **root** → **Next**
5. A window '*Pick an account*' will appear

- Click *Computer administrator* → **Create account**

Now you have created a new account. But this account is not protected by a password by default. Therefore you have to set a password for this account!

1. Click *Start* → *Control Panel* → *User Accounts*

2. A window '*UserAccounts*' will appear:

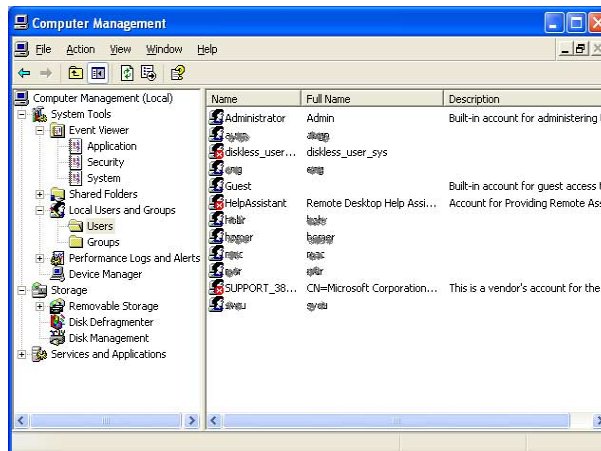
- Click **Change an account**
- Click the account you want to change → Click **Create a password**
- Type in the password, confirm it and type in a password hint → **Create Password**

Now you have for example two users with local Administrator rights, Administrator and root. Whenever the password of one of them gets lost, you can login as the other one, open the User Manager and define a new password.

The creation of the new administrator account means that the user 'Administrator' is hidden in the log in menu. You are able to log in as the user 'Administrator' by pressing twice **Ctrl+Alt+Delete** in the log in window.

14.1.2 Adding a new user in a standalone PC (method 2)

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:



- Click **Local Users and Groups**
- 3. Right mouse click **User** → Select **New User**
- 4. A window '*New User*' will appear
 - Enter the users **Full Name** and **Description** (optional) and the users password in the fields **Password** and **Confirm Password** → **Create** → **Close**

14.1.3 Adding normal users to the group NmrUser in a standalone PC

Each user who wants to run XWIN-NMR must be a member of the group NmrUser. This group is automatically created during the XWIN-NMR installation. To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
 2. A window *Computer Management* will appear:
 - Click **Local Users and Groups**
 3. Click **Groups**
 4. Highlight the group '**NmrUser**'
 - right mouse click → **Properties**
 5. A window '*NmrUser Properties*' will appear:
 - Click **Add**
 6. A window '*Select Users*' will appear:
 - Click **Advanced** → Click **Find Now**
 - highlight every name you want to be a member of NmrUsers
 - Click **OK** → **OK**
 7. Close the window '*NmrUser Properties*' by clicking **OK**
- or:*
1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
 2. A window *Computer Management* will appear:

- Click **Local Users and Groups**
- 3. Click **User**
- 4. Highlight the user '**root**'
 - right mouse click → **Properties**
- 5. A window '*root Properties*' will appear. Open the folder *Member of*.
 - Click **Add**
- 6. A window '*Select Groups*' will appear:
 - Click **Advanced** → Click **Find Now**
 - highlight group you want to be a member of
 - Click **OK** → **OK**
- 7. Close the window '*NmrUser Properties*' by clicking **OK**

14.2 User Management in a Domain PC

14.2.1 Adding a second user with Administrator rights in a domain PC

The group '*domain admins*' are automatically a member of the local group '*administrator*' so it is not necessary to create a second user with administrator rights.

14.2.2 Adding a local user in a domain PC

1. Log in as Administrator
2. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
3. A window *Computer Management* will appear:
 - Click **Local Users and Groups**
4. Highlight '*User*'
 - right mouse click → **New User**
5. A window '*New User*' will appear
 - Enter the users **Full Name** and **Description** (optional) and the users pass-

word in the fields **Password** and **Confirm Password** → **Create** → **Close**

6. Highlight the user you had just create
 - right mouse click **Properties**
7. A window '*<Username> Properties*' will appear:
 - Click **Member off** → **Add**
8. A window '*Select Groups*' will appear:
 - Click **Advanced** → Click **Find Now**
 - highlight every name you want to be a member of NmrUser
 - Click **OK** → **OK**
9. Close the window '*<Username> Properties*' by clicking **OK**

Click **Start** → **Shut Down**

Select **Log off Administrator**

Click **OK**

Press **CTRL+ALT+DEL**

→ Now you can log on as the new user

14.2.3 Adding normal users to the group NmrUser in a domain PC

Each user who wants to run XWIN-NMR must be a member of the group NmrUser. This group is automatically created during the XWIN-NMR installation. To add a user, log in as Administrator (otherwise you will be asked for the administrator password during the process) and proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:
3. Click **Local Users and Groups**
 - Click **Groups**
4. Highlight the group '*NmrUser*'
 - right mouse click → **Properties**

5. A window '*NmrUser Properties*' will appear:
 - Click **Add**
6. A window '*Select Groups*' will appear:
 - Click **Advanced** → Click **Find Now**
 - highlight every name or group you want to be a member of NmrUser
 - Click **OK** → **OK**
7. Close the window '*<Username> Properties*' by clicking **OK**

14.2.4 Adding a global group to the local group NmrUser in a domain PC

Users who want to use XWIN-NMR must be member of the group NmrUser. In a Domain scenario we recommend to administrate users in global groups which are added to the local group NmrUser. Proceed as follows:

1. Go to the icon **My Computer on the desktop** → right mouse click **Manage**
or: Open the Microsoft Explorer → Go to **My Computer** → right mouse click **Manage**
2. A window *Computer Management* will appear:
3. Click **Local Users and Groups**
 - Click **Groups**
4. Highlight the group '**NmrUser**'
 - right mouse click → **Properties**
5. A window '*NmrUser Properties*' will appear:
 - Click **Add**
6. A window '*Select Users*' will appear:
 - Select in the field '*Location*' the domain name
 - In the window '*Enter Network Password*' type in your login name and password
 - Highlight the global group you want to be a member of NmrUsers (normally this is the group '*Domain Users*')
 - Click **OK** → **OK**
7. Close the window '*NmrUser Properties*' by clicking **OK**

Part III

Tips, Tricks and Troubleshooting

Chapter 15

Troubleshooting

15.1 General checks

15.1.1 Windows XP Services

The NMR-SUITE requires the following Windows XP Services to control a spectrometer. Proceed as follows:

1. Click **Start** → **Settings** → **Control Panel** → **Administrative Tools**
2. Double-click **Services**
3. A window '*Services*' will appear:

At least the following services should appear with status **Started**:

- Bfs
- Bootparam
- Bruker FLEXlm License Server (only if the PC has a local license. If the license server is a remote machine, the FLEXlm service has to be started only there)
- Hummingbird Inetd
- Hummingbird NFS Server

- Hummingbird Port Mapper
- NuTCRACKER Service
- Schedule

Note that this list only contains the Services required for the NMR-SUITE. Several other Services are required for Windows XP and possibly for other software packages on your system.

4. If one or more of these services are not running:
 - Reboot the computer and check again
5. If rebooting does not solve the problem, then proceed as follows:

If the NuTCRACKER Service, bfs and/or bootparam are not running:

 - Re-install XWIN-NMR and DISKLESS (see chapter 11.3)

If the Hummingbird NFS Server and/or Port Mapper are not running:

 - Remove the NFS Server directory
(normally C:\Program Files\NfsSrvr.nt)
 - Re-install the NFS Server (see chapter 10.4)
6. Carefully check the NFS Server configuration (see chapter 11.6).

15.1.2 The Event Viewer

If you have any problems on your Windows XP host, it is always a good idea to look at possible Events which caused them:

1. Click **Start** → **Control Panel** → **Administrative Tools** → **Event Viewer**
2. A window 'Event Viewer' will appear:
 - Click **Application Log** to see Application Events
 - Click **System Log** to see System Events
 - Click **Security Log** to see Security Events
3. Double-click on an Event to get more information on it.
4. Note that Events do not necessarily indicate problems. In fact, there are three type of events: *Information*, *Warning* and *Error*.

To prevent the Event Log from getting full we recommend to do the following:

5. Click on one of the three Log's, e. g. **System Log** → **Action** → **Properties**

6. A window 'System Log Properties' will appear:
7. Set the 'When maximum log size is reached' to one of the following:
 - **Overwrite Events as Needed**
 - **Overwrite Events Older than 7 Days**

15.2 XWIN-NMR does not start

If XWIN-NMR does not start, you should first look for an error message in the window where the XWIN-NMR startup messages appear. Then check if you have one of the following problems:

- XWIN-NMR does not start, no error message:
→ Click the Exceed button on the Taskbar.
- A window 'Choose Server or File' appears:
The file `license.dat` was not found. You might have one of the following problems:

The Flexlm license manager is not installed

→ Install Flexlm license manager from the NMR-SUITE CDROM

`license.dat` has been deleted or renamed

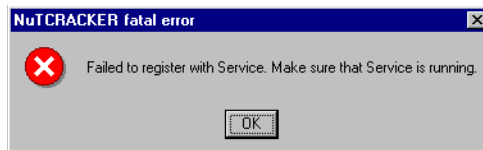
→ Setup the file `license.dat` as described in chapter 12.2.4.

`license.dat` has a (hidden) extension `.txt` or `.example`

→ Rename the file to `license.dat`

!

- 'NuTCCRACKER fatal error; failed to register this Service'



Click **OK**, then just try starting XWIN-NMR again, it might work the second or third time. This error appears if XWIN-NMR started immediately after booting the PC and so the Nutcracker Service is not yet running. If this does not work:

1. Click **Start** → **Control Panel** → **Administrative Tools**

2. Double-click **Services**

3. A window 'Services' will appear:

select **Nutcracker**, click **Start**

If the service Nutcracker does not start, there might be 2 different causes:

a) Certain system software was installed after installing an Windows XP Service Pack

→ re-install the Service Pack

b) XWIN-NMR was removed and re-installed without rebooting the computer in between.

→ Remove XWIN-NMR, reboot and re-install XWIN-NMR

- If hostid '0' or 'ffffff' occurs:

You may run Windows XP and your network-adaptor has no link to the network. Establish an link to the network or install the

NWlink IPX/SPX/NetBIOS Compatible Transport Protocol:

a) Click **Start** → **Control Panel** → **Network Connections**

b) Right-click **Local Area Connection xxx**

c) Click **Properties** → **Install...** → **Protocol** → **Add**

d) The *Select Network Protocol*-menu will appear after some seconds. Click **NWlink ...** → **OK**

e) After some seconds the Properties-menu will reappear → Click **Close**

- '*Cannot connect to license server... WinSock Error code...*'

The file `license.dat` was found, but Flexlm does not run. Maybe:

a) Flexlm is not installed: → Install Flexlm from the NMR-SUITE CDROM

b) the Service (Bruker) Flexlm license server is not running:

→ Click **Start** → **Control Panel** → **Administrative Tools**

- Double-click **Services**

- A window 'Services' will appear:

- Select **Flexlm...**, click **Start**

- *'Server node is down or not responding (-96,379)'*

The server could not answer because he is down, the entry <SERVER-NAME> in 'license.dat' is wrong or the server has been wrong configured:

→ Check if the server in the 'license.dat' file is down:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**

- type '**ping** <SERVER-NAME>' and check if the correct reply occurs:

- a) A reply like this:

*Reply from <SERVER_IP_ADRESS>: bytes=32 time<10ms
TTL=128* shows that the server is okay.

- b) A reply like this: *'Request timed out'* shows that the server is down

- c) A reply like this: *'Bad IP address <SERVER-NAME>'* shows that the <SERVER-NAME> is wrong or the server is not correctly configured.

→ Check if the entry of the server in the 'license.dat' file is wrong (wrong name, blanks, ...), if so correct it.

→ Check if the server has a wrong configuration, e. g. TCP/IP protocol or NetBIOS network service is not installed. For this you should have a look at:

- **Start** → **Control Panel** → **Network Connections**

- Click on the LAN entry of your ethernet card → **File** → **Settings**

- A window *'Local Area Connections Properties'* will appear

- Look if there is an entry *'Internet Protocol (TCP/IP)'*

- Yes? click on it to highlight the entry → **Properties**

- No? see 5.1.1

- A window *'Internet Protocol (TCP/IP) Properties'* will appear

- Click on **Advanced**

- A window *'Advanced TCP/IP Settings'* will appear

- make sure that the entry *'Enable NetBIOS over TCP/IP'* is enabled

Also click:

- **Start → Control Panel → Administrative Tools**
- Double-click **Services**
- A window 'Services' will appear:
make sure that **server** and **TCP/IP NetBIOS** have the status 'started'

- *'Failed to register Kernel Service'*
the Service Nutcracker Kernel is probably not running:
→ Click **Services** in the **Control Panel**, select **Nutcracker**, click **Start**

- *'Cannot find resolution file'*
→ Reboot the computer and try again

- If you get the following error message:

*'Xcpu: Cannot get visual class PseudoColor
Please configure your X-Server to
PseudoColor and 8 bit per plane
visual class 'TrueColor' not supported.
Please configure 8 bit per plane'*

!

The Color Palette of the Display Properties is probably not set to 256 colors.
Click **Start → Settings → Control Panel → Display → Settings**, Select **256 Colors** and reboot the computer (see also chapter 3.4).

- If you get the following error message:
*XWIN-NMR requires that a suitable
X Server is installed
Program is exiting...
Hit ENTER to continue ...*

Either there is no Xserver installed, in this case refer to chapter 10.3, or the au-

automatic start of the X-server does not work properly, follow the instructions in chapter 11.6

- *'Invalid license key (inconsistent license key)'*

The file `license.dat` might contain one of the following errors:

- The `hostid` in the `SERVER` line is wrong
 - The `FEATURE` line contains the wrong license key, the wrong date and/or the wrong number of licenses
 - The `hostid` is appended at the end of the `FEATURE` line (this is correct for *Node Locked* licenses but not for *Floating* licenses, see chapter 12.1)
-
- *'Invalid data returned from license server'*
 - Hostname in the file `license.dat` is incorrect
-
- *'Invalid host'*
 - The file `license.dat` contains additional characters at the end of the `FEATURE` line (after “”)

For more information on the Flexlm license manager:

Click **Start** → **run** enter `c:\flexlm\bruker\help\index.htm` click **OK**

15.3 XWIN-NMR hung up

If XWIN-NMR hung up, please try the following steps. These steps are increasingly drastic.

1. Press the **Esc** key

this will not kill XWIN-NMR and might enable input again

2. Do a 'graphics restart' in the following way:
 - a) Press **CTRL+SHIFT+ESC** to start the Task Manager
 - b) Click **Processes**
 - c) Click **xcpu.exe**
 - d) Click **End Process**

Note that a graphics restart cannot be done by typing CONTROL Backslash in the shell window like it is possible on a UNIX workstation.

3. Kill XWIN-NMR in the following way:
 - a) Press **CTRL+SHIFT+ESC** to start the Task Manager
 - b) Click **Applications**
 - c) Click **XWIN-NMR 3.x**
 - d) Click **End Task**

4. Kill XWIN-NMR in the following way:
 - a) Find the shell window from which XWIN-NMR was started
 - b) Click the **X** button in the upper right corner

15.4 Communication problems between PC and CCU

If the acquisition (**zg**, **gs**, **wobb**) and/or the configuration (**cf**) fails, you might have a communication problem between the PC and the spectrometer CCU.

15.4.1 Hardware related problems.

Check if the Ethernet cable between the PC and the CCU is properly connected.

→ Remove and re-connect the Ethernet cable.

5. If your spectrometer has a CCU/8 or older it must be upgraded with special PROMS in order to boot from a Windows XP computer. There are two different sets of PROMS, one for CCU/4-6 (H5323+H5324) and one for CCU/8 (H9133+H9134).
6. Does the connection light come on if you connect CCU and ethernet board in the PC?

a) If the light is off

The connection light is one of the three LEDs that most Ethernet cards have. One of them, usually in yellow, lights up the same moment that both ends of the respective cable are connected to life devices like a hub or wall socket or a computer.

- Check the cable or the Ethernet card; with some cards you need to reboot the PC with CCU and Ethernet-board being connected to make the initial connection. If the PC is started without any cable connected to the board some configurations will disable the card unless configuration takes place (makes sense for unused cards, however forces us to re-boot more often than we might want to).
- If you have a CCU 9: try 'the other' 10baseT slot on the board. One of the slots has two lines crossed for an inter-hub connection or a direct computer-to-computer connection, the other has a straight connection on all lines. The straight cables go into the lower slot on the board; crossed cables go into the upper slot of the two 10baseT slots on the CCU board; Make sure you are connected to the correct socket.
- In some cases the auto-negotiate protocol of certain cards doesn't work. That means CCU can't find out whether to go for 10baseT or 100baseT. Some of the newer Ethernet cards allow you to switch the auto-negotiate off. Software configuration allows you to set a fixed speed of 10. In some cases you can also force a card into 10Mbps by putting a hub (a 10Mbps hub!) between PC and CCU. The hub will tell the card to switch to 10Mbps and CCU gets around auto-negotiate, too.

If the light still doesn't come on, please connect the Ethernet board with some operational network (e.g. corporate network). If you get a physical connection (light goes on) obtain a temporary IP address for the PC and install the card, network, netmask, DNS etc to the point where you see the rest of the company through the 'network neighborhood' of your PC. This will make sure that your card works at all. Then switch back to the IP/netmask for speed and reboot PC. Is the light on? If not, get a new Ethernet card.

b) If the light is on:

At this point you know that the physical connection is intact (that is: the connection light on the PC's Ethernet board came on). There are two possibilities to check from here:

- CCU is indeed booting OK, yet you can't access it for some reason.
- CCU really does not boot and you have to find out why.

Before you proceed you might want to quickly check the settings in NFS Maestro. Call it from the Control Panel (HCL NFS Server) and you need to see the configuration given in chapter 11.6. If settings have to be altered, do this, reboot the PC and then the CCU before checking again.

- The minimum test is this: Try to *ping spect* and then to *telnet spect* (see chapter 13.2). Here is how to proceed:

If you can `ping` and `telnet` and get `spect`'s login prompt you should be able to run XWIN-NMR from here. You are all set.

If you can `ping` but cannot `Telnet` to CCU the physical connection is all right but CCU doesn't boot. Please connect a monitor cable to CCU and open a HyperTerminal connection. HyperTerminal is Windows's text terminal emulator and it comes with every copy of Windows. The details are in chapter 15.4.5

If you can't even `ping` CCU try a new Ethernet cable and if it still doesn't work try another type of Ethernet card.

15.4.2 Software related problems

Please check if the required Services are running as described in chapter 15.1.1.

15.4.3 View the output of the CCU console

In order to view the output of the spectrometer CCU, you must connect the COM2 port of the PC to `tty00` of the CCU. For CCU/9, you need a cable with a round `rs232` plug on the CCU side (order number HZ04161/A). For `CCU < 9` you need a cable with a 9-pin `rs232` plug on the CCU side (order number HZ10034/A). The hyper terminal application can be used to make the output of the CCU visible on the PC (this has the same function as `cu` and `kermi t` on UNIX systems).

15.4.4 Configuration of HyperTerminal

1. Click **Start** → **All Programs** → **Accessories** → **Communications** → **HyperTerminal**
2. If you do this for the first time HyperTerminal will ask for some informations in

the window '*Location Information*'. Type in your ZIP-code and click **OK**

3. A window '*Phone And Modem Options*' will appear → **OK**

Then establish a new connection:

4. A window '*Connection Description*' will appear:

- a) In the Field **Icon**: click any icon you decide for
- b) In the field **Name**: enter **CCU**
- c) Click **OK**

5. A window '*Connect to*' will appear:

- a) Click in the field **Connect using**: select **COM2**
- b) Click **OK**

6. A window '*COM2 Properties*' will appear:

- a) Click in the field **Bits per second** and select **9600**
- b) Click in the field **Flow Control** and select **Xon/Xoff**

(the other settings remain unchanged: Data bits 8, Parity None, Stop bits 1)

- c) Click **OK**

→ the output of the CCU will appear in the window '*CCU Hyper Terminal*'

7. Click **File** → **Save**

8. Click **File** → **Exit**

9. Answer the question '*Are you sure you want to disconnect now?*' with **Yes**

15.4.5 Usage of Hyper Terminal

1. Click **Start** → **All Programs** → **Accessories** → **Hyperterminal** → **CCU.ht**

2. A window CCU Hyper terminal will appear in which you see the output of the CCU.

If the CCU is booted, you will see a login prompt and you can log in as root. If the CCU is not booted you can push the reset button on the CCU and view the boot process. The boot process is shown below. The messages '*Fast ethernet...*' only occur for CCU/9 and indicate whether you have a 10 MBit/s or 100 MBit/s ethernet connection. Note that a UNIX pathname for the DISKLESS program is shown. Do not worry about this, it is automatically interpreted as an Windows XP path like: C:\Bruker\Diskless...

```
Autoboot:  Waiting    to    load    bfs()/usr/diskless/cli-
```

```

ents/spect/root/unix.r4600_std (
CTRL-C to abort)
loading

Fast ethernet (FEN): 100 MBit/s, half duplex
---1---
Obtaining /usr/diskless/clients/spect/root/unix.r4600_std
from server 'hostname'
833328+107984+827152 entry: 0x80021000
CPU: MIPS .... Processor Chip Revision: ...
FPU: MIPS .... Floating Point Unit [CP1] Revision: ...

RISC/os Release 4_52 mips Version UMIPS
Total real memory = 16777216
Available memory = 14360576
Root on nfs file :,Swap on nfs f
Fast ethernet (FEN) : 100 MBit/s, half duplex
---2---
hostname: spect
domainname: software.bruker.de
---3---
Root fstype nfs
Available memory = 12713984

---4---
The system is coming up. Please wait.
/etc/init.d/sym_install start
/etc/init.d/sym_install calls sym_install
Adding swap device /swapfile
Fast ethernet (FEN) : 100 MBit/s, half duplex
Internet daemons: portmap inetd.
NFS daemons: nfsd biod lockd statd.
/tmp: Permission denied
/var/tmp: Permission denied
The system is ready:

```

spect Console login:

Booting might hang, stop (and print an error message) or go into an endless loop at one of the positions 1 through 3. This might be caused by one of the problems mentioned below. Check the indicated files and correct them if necessary or per-

form the indicated steps.

- a) If booting stops at position ---1--- and you get the messages:

```
Fast ethernet (FEN): 100 MBit/s, half duplex
No server for /usr/diskless/clients/spect/root/un-
ix.r4600_std
BRUKER CCU R4600 Monitor
Version 5.40 MIPS OPT Wed Jun 11 19:30:43 MSZ 1997 root
Memory size: 16777216 (0x1000000) bytes, 16 MB
Icache size: .... (....) bytes
Dcache size: ..... (....) bytes
>>
```

then you might have one of the following problems:

- The Service *bfs* not running:

Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **bfs** → **Start**

- The Diskless package is not installed (see chapter 5.6)
- The ethernet cable between PC and CCU allows no data throughput:
 - check the connection between the cable and the PC/CCU
 - check if the correct ethernet card is connected
 - check the configuration of the ethernet port (see chapter 5.1)

- b) If booting stops at ---2--- you may have one of the following problems:

- The Service *bootparam* is not running:

Click **Start** → **Control Panel** → **Administrative Tools** → **Services** → **bootparam** → **Start**

- The file `C:\Windows\system32\drivers\etc\Hosts` is wrong:

It should contain the following entries:

```
149.236.99.1 ASP_ST2
149.236.99.99 spect
```

Be sure that 'spect' is the first entry after the number in this line

- c) If booting stops at ---3--- you might have the following problem:

- The file `c:\Bruker\Diskless\WinApp\bootparams` is wrong.
For a default installation it must contain the lines:

```
#
spect root=ASP_ST2:C:/Bruker/Diskless/clients/spect/root \
    swap=ASP_ST2:C:/Bruker/Diskless/clients/spect/swap \
    dump=ASP_ST2:C:/Bruker/Diskless/clients/spect/dum
```

For a custom installation the path of Diskless can be different!

d) If booting hangs at ---3--- in a loop and you get the messages:

a) like this:

```
domainname: software.bruker.de
mount root ASP_ST2:C:/Bruker/Diskless/clients/spect
/root failed, rpc status 15
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have one of the following problems:

- The Service Hummingbird NFS Server is not running
Click **Start** → **Control Panel** → **Administrative Tools** → **Services**
→ **Hum. NFS Server** → **Start**
- The path C:\Bruker\Diskless\clients\spect is not exported
(see chapter 10.5).

b) like this:

```
domainname: software.bruker.de
mount root ASP_ST2:c:/Bruker/Diskless/clients/spect
/root failed, rpc status 2
PANIC: vfs_mountroot: cannot mount root
syncing disks... done
```

then you might have the problem that the drive letter of the diskless installation is written in lower case (maybe caused by a custom installation). To solve the problem you can either

- De-install Diskless and use for the new installation 'typical' or make sure that the drive letter is upper case

or

- Open the file

```
c:\Bruker\Diskless\WinApp\bootparams
```

and change all drive letters to upper case

- c) If booting stops at ---4--- and you get messages like this:

```
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
touch: /etc/mtab cannot create
mount: /etc/mtab: No such file or directory
<date> INIT: warning: /etc/ioctl.syscon does not exist, default settings assumed
<date> INIT: Can't open /etc/ioctl.syscon. errno: 13
<date> INIT: Cannot create /etc/utmp
<date> INIT: failed write of utmp entry: " "
```

Please check diskless tree permissions and NFS User- and Group-Mappings (see Chapter 11.8)

- d) If you see the message:

mount dumpfile ASP_ST2:C:/Bruker/Diskless/clients/spect/dump failed
during the boot process, you can ignore this. The CCU will boot anyway.

3. Click **File** → **Exit** to finish your Hyper Terminal session.

15.5 Troubleshooting for NMR-GUIDE

If you have some trouble with your installation of the NMR-GUIDE, e. g. the 'gserver' do not start, please check the following :

1. Check for the NMR-GUIDE password (see chapter 12)

Edit the file C:\flexlm\Bruker\licenses\license.dat and check whether there is a FEATURE NMRGUIDE line. If not, enter the FEATURE line or apply for a password at

license@bruker.de

2. Check for all necessary components

- Internet Explorer ≥ 5.0 (see chapter 7)
- Web server (see chapter 8)

3. Install the NMR-GUIDE program for the NMR-SUITE 3.5 CD once again. (This is necessary, because installation of the operating system components might have overwritten certain registry keys that are set during the NMR-GUIDE installa-

tion.)

4. Now try the NMR-GUIDE again
5. If your problem still exists please de-install the Apache HTTP Server (see chapter 8), reboot and install it and the NMR-GUIDE again (reboot once again)

15.6 Bruker Service tools

Several tools for checking the spectrometer hardware are delivered with the NMR-SUITE. This includes tools for BSMS, HPPR, ACB, GRAD, HPCU, RX22. You can start a service tool as follows, for a full description see chapter 13.3:

1. Double-click the icon **Bruker Utilities** on the desktop
2. A window will appear with the icons Service tools, Test Tools etc.:
 - a) Double-click **Service Tools** to get a list of service tools
 - b) Double-click **Test tools** to get a list of test tools
3. A windows with the available tools will appear:
 - Double-click any icon to start the corresponding tool

15.7 Windows XP Service Pack

All PC's delivered by Bruker BioSpin have the latest Service Pack installed. It can also be downloaded from the Microsoft Web pages www.microsoft.com or www.microsoft.de.

For installation just follow the given instruction on the screen.

Under Windows XP it is not necessary to reinstall the service pack after e. g. configuring the network.

During the installation, you might get the message that files were detected which are not the original Windows XP files and which are also part of the Service Pack. Sometimes, these files are even newer than the ones in the Service Pack. This typically happens when you installed recent driver software. You are asked if these files should be overwritten. Bruker BioSpin recommends to answer this question with **No**, unless you are sure you want to update this file from the Service Pack.

15.8 Disk full or fragmented

If you have disk space problems, have a look at the Windows XP Online help:

Click **Start** → **Help** → **Index**

enter **increasing disk space** choose one subentry and click **Display**. If you want to defragment your disk see chapter 19.3. Note that NTFS partitions, which are required for the NMR-SUITE, suffer much less from fragmentation than FAT partition.

Furthermore, you might have to remove XWIN-NMR data, e.g.:

1. Delete imaginary data using the **deli** command

They are no longer needed for spectra which have been phase corrected.

2. Delete processed data using the **delp** command

They can always be retrieved by reprocessing the data.

3. Delete raw data with the **del** command

Please make sure you have a backup of the data.

15.9 Creating an Windows XP Boot Disk

You can use a Windows XP bootable disk to start the operating system on a computer running Windows XP. Use the procedures in this article to work around the following boot issues:

- Damaged boot sector.
- Damaged master boot record (MBR).
- Virus infections.
- Missing or damaged `ntldr` or `ntdetect.com` files.
- Incorrect `ntbootdd.sys` driver.

You cannot use the Windows XP boot disk to help resolve the following issues:

- Incorrect or damaged device drivers that are installed in the System folder.
- Boot issues that occur after you see the Windows XP startup (Osloader) screen.

15.9.1 PC is not booting from floppy?

In case it is not possible to boot the PC from a bootable floppy, this possibility might be disabled in BIOS. The following description shows how to enable the boot-from-floppy feature on a hp workstation xw4100 PC. On other PC's the procedure might be slightly different.

1. During boot time cancel the boot process and go into BIOS

On different PCs there are different ways to do this, for example, on some PCs the boot sequence is interrupted with the **Delete** key rather than with the **F2** key.

2. Go to section

Security → Boot Devices Security

3. Set *Floppy* to **Enabled**

Note: It is recommended to disable the boot-from-floppy feature after the boot process is done!

If it is enable, it is possible to get very easily a boot virus into BIOS, that can make your PC defective!

Another small advantage is, that if the BIOS feature above is enabled and a 'normal' floppy is inside the drive, booting the PC will stop and showing the information that a non bootable floppy is inside. If it is disabled booting the operating system will work with or without floppy.

15.9.2 Floppy boots Operating System from hard disk

You can create an Windows XP Boot Disk by formatting a floppy from within Windows XP and copying the following files from the root of an Windows XP boot partition (e.g. C:) to the floppy (Special note: the boot partition is the first partition which is read by bios. This is normally but not necessary the partition 'c:'. If you installed Windows XP on a different partition e.g. 'd:', the following files are anyhow on 'c:').

- ntldr
- ntdetect.com
- boot.ini

If you are using SCSI disks with the SCSI BIOS disabled then also copy the file:

- ntbootdd.sys

a) Create a Boot Floppy Disk with the command prompt

Copy these files with command prompt is easier to describe than with the Windows explorer, because these are critical system files that are normally not shown in the explorer window.

1. Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
2. Type **c:**
3. Type **dir /ah** → you should see the necessary files
4. Type **xcopy /h boot.ini a:**
5. Type **xcopy /h ntldr a:**
6. Type **xcopy /h ntdetect.com a:**
7. If necessary (see above) type **xcopy /h ntbootdd.sys a:**

Now you can boot your PC from the Boot floppy. Be aware that this will only work if Windows XP is still on the hard disk. If Windows XP is not available or corrupt it must be repaired again from CDROM or from floppy.

b) Create a Boot Floppy Disk with the Windows Explorer

1. Format a floppy disk by using the Windows XP format utility.
2. Copy the `ntldr` and the `ntdetect.com` files from the I386 folder on the Windows XP Setup CD-ROM, Windows XP Setup floppy disk, or from a computer that is running the same version of Windows XP as the computer that you want to access with the boot floppy.
3. Copy the `boot.ini` file from a computer that is running Windows XP.
Or create a `boot.ini` file, and then modify it to match the computer that you are trying to access. The following example works for a single-partition IDE drive with Windows XP installed in the `\Windows` folder, but the exact value in the `[operating systems]` section depends on the configuration of the Windows XP computer that you are trying to access:

```
[boot loader]
```

```
timeout=30
```

```
Default= multi(0)disk(0)rdisk(0)partition(1)\windows
```

```
[operating systems]
```

```
multi(0)disk(0)rdisk(0)partition(1)\windows="Windows XP"
```

If your computer boots from a SCSI hard drive, you may need to replace the

multi(0) entry with scsi(0). If you are using scsi(x) in the `boot.ini` file, copy the correct device driver for the SCSI controller in use on the computer to the root of the Setup disk, and then rename it `ntbootdd.sys`. Change the disk(0) number to represent the SCSI-ID of the hard drive you want to boot to. If you are using multi(x) in the `boot.ini` file, you do not need to do this.

4. Start your computer by using the floppy disk, and then log on to Windows XP.

15.10 Backup of Windows XP and the NMR-SUITE

The standard backup programs under Windows XP is called **ntbackup** which can be started by clicking:

Start → All Programs → Accessories → System Tools → Backup

Under Windows XP ntbackup is possible to use ZIP, tape and external hard disks as backup media.

You cannot choose a CD-R, CD-RW, or DVD-R device because ntbackup.exe does not support backing up to these devices. The **Removable Storage Management (RSM)** does not have the ability to recognize these three devices as backup pool media. RSM regards CD-R, CD-RW, or DVD-R as just a file system-capable media type, but the Windows file system does not support formatting these media types. When it attempts to write an RSM free label, RSM does not succeed because the disc appears to be write protected. This means that RSM treats CD-R, CD-RW, or DVD-R media as a read-only media type even if you add them to the ntbackup media pool. Before you buy a tape drive, make sure it is compatible with your PC's interface(s); IDE and/or SCSI.

Bruker BioSpin recommends to make a regular backup of the partition(s) on which Windows XP and the XWIN-NMR are installed.

15.10.1 Complete Backup of the PC

1. Click **Start → All Programs → Accessories → System Tools → Backup**
→ a window *backup* will appear
2. Click **Welcome → Backup Wizard**
→ a window *Backup Wizard* will appear → **Next**

3. Enable *Backup everything on my computer* → **Next**
4. Choose the media drive you want to store the backup → **Next**
5. Click '*Finish*' to start the backup

15.10.2 Backup of specific directories

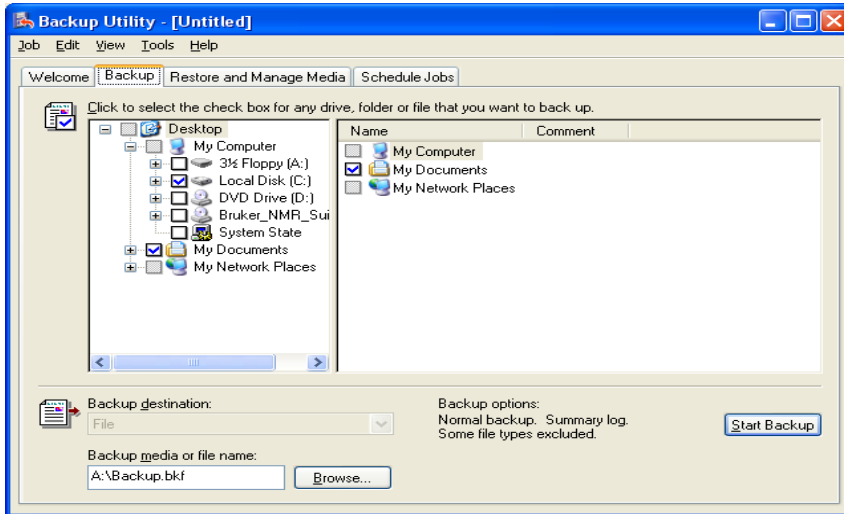
1. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **Backup**
→ a window *backup* will appear
2. Click **Backup**
→ all available drives will appear
3. Choose the directory you want to backup. Click the check box left of the directory to select the entire path for backup → a tick will appear in the check box
4. Choose the *Backup media or file*
5. Click **Start Backup**
6. A window *Backup Job Information* will open
7. Click **Start Backup**

15.10.3 Frequent backup of specific directories

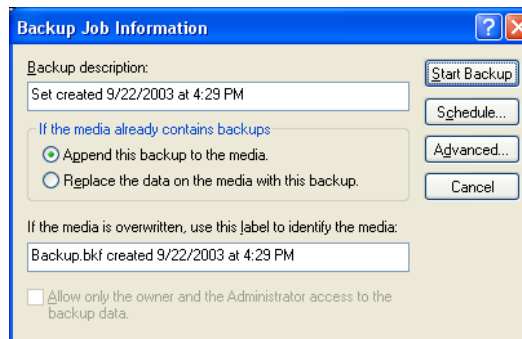
If you commonly use Ntbackup to back up a single folder, you might want to create a simple batch file. Suppose you would like to make a daily backup of a directory:

1. Choose the path of the file as describe above

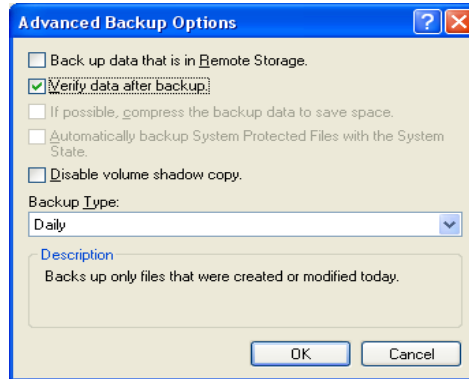
2. Click **Start Backup**



3. A window *Backup Job Information* will open



4. Click **Advanced**



5. Click the arrow at the right of the field *Backup Type* and choose **Daily**

6. Click **OK** → Click **Start Backup**

15.11 Security check of a Windows XP system

Microsoft offers a tool for free download that checks your PC for security leaks. The result is listed with an evaluation of the different topics. For further details check the following Microsoft website.

<http://www.microsoft.com/technet/treeview/default.asp?url=/technet/security/tools/Tools/mbsahome.asp>

15.12 Restore the Operating System to a Previous State in Windows XP

Use the System Restore tool in order to return your computer to a previous working state. The System Restore takes a 'snapshot' of critical system files and some program files and stores this information as 'restore points'. You can use these 'restore points' to return Windows XP to a previous state.

15.12.1 Using System Restore to Restore Windows XP

- **Windows XP Does Not Start**

If Windows does not start, restart Windows by using the 'Last Known Good Configuration' feature:

1. Start the computer and then press the **F8 key** when Windows begins to start. The 'Windows Advanced Options' menu appears.
 2. Select 'Last Known Good Configuration' (your most recent settings that worked), and then press **ENTER**.
 3. If a boot menu appears, use the ARROW keys to select **Microsoft Windows XP**, and then press **ENTER**. Windows XP restores the computer to the most recent restore point.
- **Windows XP Does Start**
 1. Log on to Windows as an Local Administrator.
 2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.
 3. A window *Welcome to System Restore* appears, click **Restore my computer to an earlier time** (if it is not already selected) → click **Next**.
 4. A window *Select a Restore Point* appears. Click the most recent system checkpoint in **On this list**, click a **restore point** list → click **Next**.
 5. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.
 6. On the Confirm Restore Point Selection page, click **Next**. System Restore restores the previous Windows XP configuration, and then restarts the computer.
 7. Log on to the computer as an administrator. A window *The System Restore Restoration Complete* will appear → Click **OK**.

15.12.2 Troubleshooting

It could happen that you restore Windows XP to a previous configuration that you do not want. To undo the restoration:

1. Log on to Windows as an administrator.
2. Click **Start** → **All Programs** → **Accessories** → **System Tools** → **System Restore**. System Restore starts.
3. A window *Welcome to System Restore* appears. Click **Undo my last restoration** → **Next**.
4. A System Restore message may appear that lists configuration changes that System Restore will make → click **OK**.

5. On the **Confirm Restoration Undo** page, click **Next**. System Restore restores the original Windows XP configuration, and then restarts the computer.
6. Log on to the computer as Administrator. A window *The System Restore Undo Complete* appears → Click **OK**.

15.13 Turn on and turn off System Restore in Windows XP

The 'System Restore' is the feature that allows a computer system to be 'rolled back', or restored, to a point in time before certain events took place, for example, prior to specific software or hardware installations. System Restore monitors changes to the system and some application files, and automatically creates restore points. You can also create your own restore points at any time.

In Windows XP the 'System Restore' is enabled by default.

15.13.1 Turn on System Restore

To turn on System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to clear the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.

15.13.2 Turn off System Restore

When you turn off System Restore, all existing restore points are removed, and you are no longer able to track or undo changes to your computer. To continue to use System Restore to restore your computer to a previous state, do not turn off System Restore.

To turn off System Restore, follow these steps:

1. Click **Start** → right-click **My Computer** → click **Properties**.
2. Click the **System Restore** tab.
3. Click to select the **Turn off System Restore** check box (or the **Turn off System Restore on all drives** check box) → click **OK**.
4. Click **Yes** when you receive the prompt to the turn off System Restore.

15.14 Start the system restore tool from a command prompt in Windows XP

Windows XP includes the System Restore tool, but you cannot start the System Restore tool from a Recovery Console prompt. Because of this, it may be useful to start the System Restore tool when you are unable to start your Windows XP-based computer normally or in Safe mode.

NOTE: You must log on with administrator rights.

1. Start your computer to Safe Mode with Command Prompt.
2. At the command prompt, type

```
%systemroot%\system32\restore\rstrui.exe
```

and then press ENTER.

Follow the instructions on the screen to begin restoring your computer to a previous, functional state.

15.15 Logon problems: Last Known Good

Changes in the Registry must be made with extreme care, any mistakes can make the system unusable. Occasionally, software installations make erroneous Registry entries. If your PC does not boot any more, you can try to go back to the so-called Last Known Good, the last Registry Control Set with which the system successfully booted. Please proceed as follows:

1. Reboot and **Interrupt** the boot process hitting F8 when you see:
For troubleshooting and advanced startup of Windows XP press F8
2. Use the arrow down/up keys to select the entry '*Last Known Good*', then press **ENTER** and follow the instructions

Warning: when you reboot the computer after you installed new software, wait until all disk activity has finished, before you log on. As soon as you log on, the current control set becomes the Last Known Good and the Original Control Set (before software installation) is gone.

15.16 Boot disks for Windows XP, if the CDROM is not bootable

If your computer does support booting from a CD-ROM, or if network-based installation is available, please use those installations methods instead.

The Windows XP startup disk allows computers without a bootable CD-ROM to perform a new installation of the operating system. Setup boot disks for Windows XP are available only by download from Microsoft.

If you want to download the setup disks, the download contains only one large program file. When you execute the downloaded file, it extracts the files. There are six Windows XP Setup boot floppy disks, which contain the files and drivers that are required to access the CD-ROM drive and begin the setup process.

Note: You will need to use the Windows XP CD-ROM!

15.16.1 Downloading the Setup Disk Program File

To download the setup boot disks, please go to the Microsoft Web sites and download:

- Windows XP Professional Original Version

<http://www.microsoft.com/downloads/release.asp?ReleaseID=33291>

- Windows XP Professional Service Pack 1 (SP1)

Note: Windows XP CD-ROMs that include SP1 have the text "Includes Service Pack 1" on the CD-ROM.

<http://www.microsoft.com/downloads/release.asp?releaseid=42819>

15.16.2 Creating the Setup Disks

Note: The program creates the setup boot disks for Microsoft Windows XP. To create these disks, you need to provide six blank, formatted, high-density disks.

1. Open the **Windows Explorer** and change to directory with the downloaded program file.
2. Double-click the *program file* (e.g. WinXP_EN_PRO_BF.EXE for Windows XP Professional Original Version).
3. A info window with the License Agreement appears: Click **Yes** to confirm.
4. A command prompt appears:

This program creates the Setup boot disks for Microsoft Windows XP. To create these disks, you need to provide 6 blank, formatted, high-density disks.

Please specify the floppy drive to copy the images to:

5. Enter the letter for the floppy disk drive (typically A).
6. After you typed in the floppy disk drive letter, you see the following message:
Insert one of these disks into drive letter. This disk will become the Windows XP Setup Boot Disk.
→ Press any key when you are ready.
7. The file starts extracting and copying the files. Continue inserting the blank disks as you are prompted to do so until all six disks are created. If the process is interrupted you must run the downloaded program file again to create all six disks.

Label each disk appropriately with the number that is specified by the program!

15.16.3 Using the Setup Disks

You have created all six disks:

1. Insert the first disk in the floppy disk drive → restart the computer.
Note: The PC must be configured to boot from the floppy disk drive.
2. The setup process starts.
3. Insert the other floppy disks as you are prompted to do so.
Note: You will need to use the Windows XP CD-ROM to finish Setup.

Chapter 16

File and directory handling

16.1 Viewing and opening files/directories

Windows XP offers three different ways of finding files or directories (folders). If you want to find a specific file and you have no idea where it resides, you can use the **Search** program. If you want to get an overview over the directory tree(s), you can use **Windows Explorer** or **My Computer**.

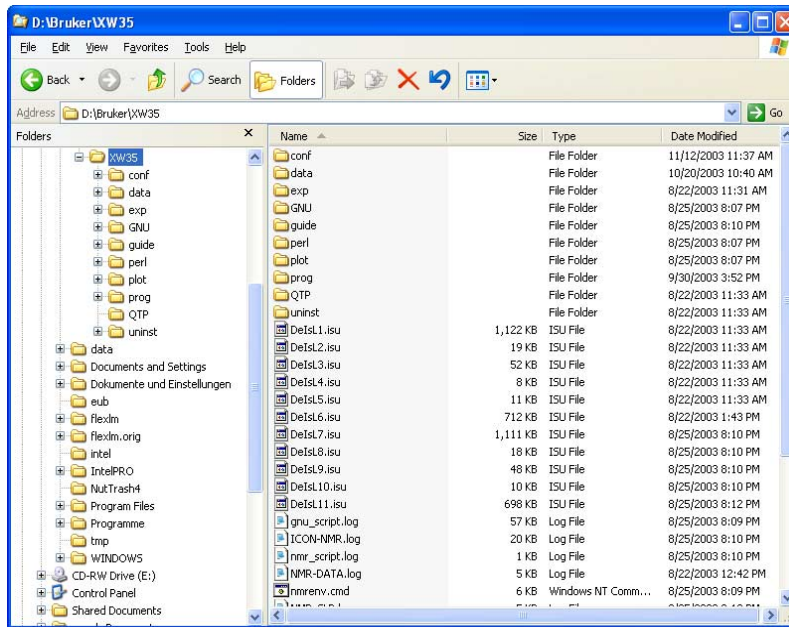
16.1.1 Windows Explorer

The Explorer provides an overview over all drives, directories and files in a two paned window.

1. Click **Start** → **All Programs** → **Accessories** → **Windows Explorer**
or right-click **Start** → **Explore**
2. A double-paned window '*Exploring*' appears
 - On the left side you see all drives and top level directories
 - On the right side you see the contents of the drive or directory which is currently selected on the left side.

A drive or directory can be expanded in the left pane by clicking on the '+' button to the left of its icon. The '+' button changes to a '-' button. When you click the

icon itself, contents of the directory will appear in the right pane. A double-click on the icon, both expands the directory and shows its contents



16.1.2 My Computer

The **My Computer** window provides an overview over all drives, directories and files. The differences under Windows XP between the **Explorer** and **My Computer** are very small. In fact you can use both windows with the same layout and handling.

1. Double-click the icon **My Computer** on the desktop
2. A window 'My Computer' will appear, showing the computer's drives:
3. Double-click a drive, e.g. (C:)
4. A window showing the contents of the top level directory on C: will appear:

Double-click any icon. Depending on the file type, one of the following will happen:

- A directory (Folder) will be opened and its contents will be shown
- An executable program will be started

- A text file will be opened using an editor (by default **notepad**)
- For an unknown file type, a window '*Open with*' will appear, showing a list of available programs

If you click a directory icon two things might happen:

- the directory contents appears in a new window
- the directory contents replaces the contents of the current window

You can configure this feature according to your preference:

- a) Double-click the icon **My Computer** on the desktop
- b) Click **Tools** → **Options**
- c) A window '*Options*' will appear:
 - Click **General** and select one of the two **options** of '*Browse Folders*'

The disadvantages of a separate window for each directory is that your screen is soon filled up with windows. However, a quick way of closing an entire hierarchy of windows is the key combination **ALT+SHIFT+F4**.

If you want the explorer layout as a two paned window, select **View** → **Explorer Bar** and enable '**Folders**'. You are not able to store this configuration, this might be the biggest difference between the **Explorer** and **My Computer**

16.1.3 Explorer and My Computer can hide file extensions

Windows XP Explorer and My Computer allow you to hide known file extensions like `.txt`, `.fm`, `.doc` etc. One of the problems when you hide them is that the editor Notepad appends the extensions `.txt` to files which do not have a known extension. For example, `license.dat` is changed to `license.dat.txt` and thereby becomes unusable. Therefore, we recommend to configure My Computer such that it shows file extensions:

1. Double-click **My Computer**
2. Click **Tools** → **Folder Options** → **View**
3. Unselect **Hide file extensions for known file types**
4. Click **OK**

This setting also applies to Explorer.

16.1.4 Search

The Windows XP Find program allows you to search files and directories according to various criteria.

Suppose you are looking for the file named `cosy`:

- a) Click **Start** → **Search** → **For Files or Folders**
(or press **F3** when the cursor is on the desktop background)
- b) Click the small arrow right of the field **Look in:** select the drive on which you expect to find the file. If you select **My Computer**, all drives will be searched.
- c) In the field **Named:** enter `cosy`
- d) Click **Find now**

All files which contain the string `cosy` in their name will appear in the result, e.g. `cosy`, `cosygs`, `pecosy`. You can directly open the file by clicking on it. Furthermore, you can also search for text files which contain a certain string if you define it in the field '*Containing Text*'. Clicking on '**Search Options**' will show you some more parameters like '*Date*' or '*Size*' which you can add in your search options

16.1.5 The Windows Command Prompt

A Windows XP Command Prompt (shell) can be opened in three ways:

- Click **Start** → **All Programs** → **Accessories** → **Command Prompt**
- Click **Start** → **Run** enter `cmd` click **OK**
- Press **CTRL+ESC** → **r** enter `cmd` click **OK**

A window will appear where you can enter Windows commands like `cd`, `dir`, `type`, `copy`, `ren`, `move`, `notepad`, `print`, `ipconfig`, `cacsls`, `telnet`, `ftp` etc.

The default Prompt is `C:\>` when the computer was booted from this drive.

16.2 File and directory permissions

Windows XP supports file level security on NTFS but not on FAT filesystems. Note that TOPSPIN can only be installed on NTFS and as such it supports file level

security.

16.2.1 Permissions and Types of Access

Folders and files can have the following permissions:

Permission	Full Control	Modify	Read & Execute	List Folder Contents ¹	Read	Write
Traverse Folder ¹ / Execute File ²	yes	yes	yes	yes	no	no
List Folders ¹ / Read Data ²	yes	yes	yes	yes	yes	no
Read Attributes	yes	yes	yes	yes	yes	no
Read Extended Attributes	yes	yes	yes	yes	yes	no
Create Files ¹ / Write Data ²	yes	yes	no	no	no	yes
Append Data	yes	yes	no	no	no	yes
Write Attributes	yes	yes	no	no	no	yes
Write Extended Attributes	yes	yes	no	no	no	yes
Delete Subfolders and Files	yes	no	no	no	no	no
Delete	yes	yes	no	no	no	no
Read Permissions	yes	yes	yes	yes	yes	yes
Change Permissions	yes	no	no	no	no	no
Take Ownership	yes	no	no	no	no	no
Synchronize	yes	yes	yes	yes	yes	yes

¹ folder permission

² file permissions

16.2.2 Changing file permissions

The permissions of a single file can be changed as follows:

1. Find the file in the Explorer (see chapter 16.1.1)
2. Right-click the file icon
3. Click **Properties**
4. A window '*Properties*' will appear:¹
 - Click **Security**
5. Highlight the user/group for whom/that you want to change the permissions
6. Click **Allow** or **Deny** to set the permissions
7. If you want to add a new user/group click on **Add**
8. A window '*Select Users, Computers or Groups*' will appear:
 - a) Select the one you are looking for **Add** → **OK**
9. Select the permissions you want to give to the new name

If you want to select special permissions, do step 1-5 then click **Advanced**

1. A window '*Access Control Settings for <filename>*' will appear:
 - Click **Permissions** → **View/Edit**
2. A window '*Permission Entry for <filename>*' will appear:
 - Click **Allow** or **Deny** of the permissions you want **OK** → **OK** → **OK**

16.2.3 Changing directory permissions

The permissions of a directory can be changed in the same way as file permissions:

In the window '*Permissions Entry for <directoryname>*' you can select in the Field '*Apply onto*' the effects of changing the permissions. Click the small arrow right of the field **Apply onto** and select the entry of your choice. You can select any combination between folder and/or subfolder and/or files **OK** → **OK** → **OK**

1. If Windows XP is installed the security section might be not displayed. If you like to see it, you have to define it in the options of Windows Explorer. Click on '**Tools**' → '**Folder Options**', click on '**View**' and disable the entry: '*Use simple file sharing (Recommended)*'

16.2.4 Read-only attribute

The problem of setting the **Read-only** attributes only in the entire directory and not in the subdirectory is solved under Windows XP:

1. Find the file or directory in the Explorer
2. Right-click its icon
3. Click **Properties**
4. A window '*Properties*' will appear:
 - a) Click the attribute **Read-only** to switch it on or off
5. A window '*Confirm Attribute Changes*' will appear where you are able to decide if your changes are set only for the entire directory or also for the subdirectories and folders.

16.3 Known Problems in XWIN-NMR for Windows XP

AU programs which were copied from another computer are sometimes not displayed properly by Notepad. This happens if they were transferred with FTP in binary mode. You can either transfer the file again using **ftp** in ascii mode or with **rcp** or you can correct the local AU program as follows:

1. **Start** → **All Programs** → **Bruker NMR Suite** → **GNU Shell**
2. **vi au_program**
in the editor window enter:

```
:set textmode
:wq!
```
3. **notepad au_program**
→ the AU program should be displayed correctly now

16.4 Compressing files and directories

16.4.1 Setting the Compress attribute

For each file and directory under Windows XP, you can set so called attributes. One of these is the Compress attribute which reduces the size considerably.

1. Right-click a file or folder in the Explorer
2. A popup menu will appear:
 - Click **Properties**
3. A window '<name> Properties' will appear:
 - a) Click **Advanced**
 - b) Enable the attribute **Compress Contents to save disk space** → OK → OK

Compressed data will be uncompressed and recompressed automatically whenever they are accessed by an application. Note that this process will take time and your application runs slower when they work on compressed data. For transferring files or directories you might want to compress/archive them in zip format using the program Winzip rather than using the Compress attribute (see chapter 19.2).

16.5 Editing text files

You might know, UNIX doesn't write Carriage Returns (CR) at the end of text lines. That means that some files we create will not display properly in an editor like notepad:

```
hardware.exam: list of all hardware detectable by 'cf' To copy one of these entries into 'hardware_list' proce
##### PN-C | PN-D | PN-E | ECL | SN | description/comment ##### Transmitter entri
0 | B-LTH100 500-600 20+40dB(1H) 20+40dB(19F) 20+40dB(3H) | W1345031 | 0 |
1H Ecoupler 300 1x20dB(1H) | W1301100 | 3 | 1H Ecoupler 300 2x20dB(1H) |
F Ecoupler 360 1x20dB(19F) | W1301247 | 3 | 19F Ecoupler 360 2x20dB(19F) |
| W1301567 | 0 | | 19F/1H Ecou.300 20+40dB(1H) 20+40dB(19F) 20+40dB(3H) |
| W1301282 | 2 | | 3H Ecoupler 400 2x20dB(3H) | | W1301283 | 0 | | 3H Ec
0 | 0 | | Tube 100 1H/19F 60Win/1000Vout | | H5342 | 0 | | Tube 200 1
Z04680 | | HPTXcus3 | | Custom3 X-BB 30Win/1000Vout | | HPTXcus4 | |
Z04680 | | SE451 400 (SE451 RG table, no Quad Mixer) | | Z03680 | | Z082811 |
| | Z082810 | | RX22 (RX22 RG via RS485, no Quad Mixer) | | Z082811 |
| | H3623 | | MC1-Mem-Ext 64kV/ch ##### PTS entries | | 00173 |
.00 MHz doubling) | | Z012209 | | PTS-6200 Trip-500 (3 outputs, 620 MHz max, 309.0
0973 | | PTS-620 1MHz (1 output, 620 MHz max, 309.00 MHz doubling) | | 01173 |
0 Sample Changer seriell | | H11080 | | B-ACS60/600 Sample Changer Oxford |
| W1100625 | | | UTU B-UT2000 (sep. unit) | | W1101054 |
```

That doesn't mean that the file is damaged, it only means that the editor cannot resolve the issue. One reason to pick wordpad as an editor is that wordpad (unlike notepad) is smart enough to render such files:


```
# hardware.exam: list of all hardware detectable by 'cf'
#
# To copy one of these entries into 'hardware_list' proceed as described:
#
# - delete all lines except the one you want to copy:
#   vi hardware.exam
#   usable vi commands: dd (delete 1 line), <n>dd (delete n lines)
#   :wq
# hardware.exam should now contain the desired entry only!
#
# - if available: insert EC-level and SN to keep data up to date:
#   vi hardware.exam
#   insert EC-level and serial number
#   :wq
#
# - move hardware.exam into instrument directory:
#   cd `cat curinst`
#   mv ../hardware.exam .
#
# - insert desired entry into hardware_list:
#   su (become superuser)
#   cp hardware_list hardware_save (make backup)
#   vi hardware_list
#   move cursor into line where you want to insert the new entry
#   :r hardware.exam (insert file)
#   :wq
#
# finished: hardware_list should now contain the new entry.
#
#####
#
# PN-C | PN-D | PN-E | ECL | SN | description/comment
#
# Transmitter entries
#
# | W1301248 | 0 | B-LT3-S 20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
# | W1301642 | 0 | B-LT4-S 20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
# | W1301242 | 1 | B-LT4 no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)
# | W1301242 | 2 | B-LT4 20+40dB(X) 20+40dB(1H) 20+40dB(19F) 20+40dB(3H)
# | W1301240 | 1 | B-LT5 no att.(X) 2x20dB(1H) 2x20dB(19F) 2x20dB(3H)
```

For Help, press F1

Thus, if you see displays like the notepad-example above, please try a smarter editor: Wordpad comes with every Windows and those that have MS Word can of course use Word to edit files in luxury.

Chapter 17

Plotting and Printing under Windows XP

17.1 Differences between UNIX and Windows XP

17.1.1 Exchange of XWIN-NMR data between Windows XP and UNIX

XWIN-NMR under Windows XP can read data which have been created with XWIN-NMR under UNIX and vice versa. However, Windows XP data can only be read with XWIN-NMR 2.5 or newer under UNIX. Earlier versions of XWIN-NMR cannot read data created under Windows XP.

17.1.2 Plotting and printing

Under UNIX, printers drivers are delivered with the NMR-SUITE and printers can be installed with the XWIN-NMR command **cfpp**.

Under Windows XP, all common printer drivers are available and printers are installed with the Windows XP **add printer** tool (see chapter 6.1). When a printer is installed under Windows XP, it can be used for plotting from XWIN-NMR and XWIN-PLOT.

The default printer and plotter for XWIN-NMR are defined during the configuration

of XWIN-NMR by **expinstall** (see chapter 13.1.1).

An extraordinary print device in the actual dataset which is in XWIN-NMR on the screen is defined as below:

a) Enter: **edo**

Click the small arrow button to the right of the field CURPLOT

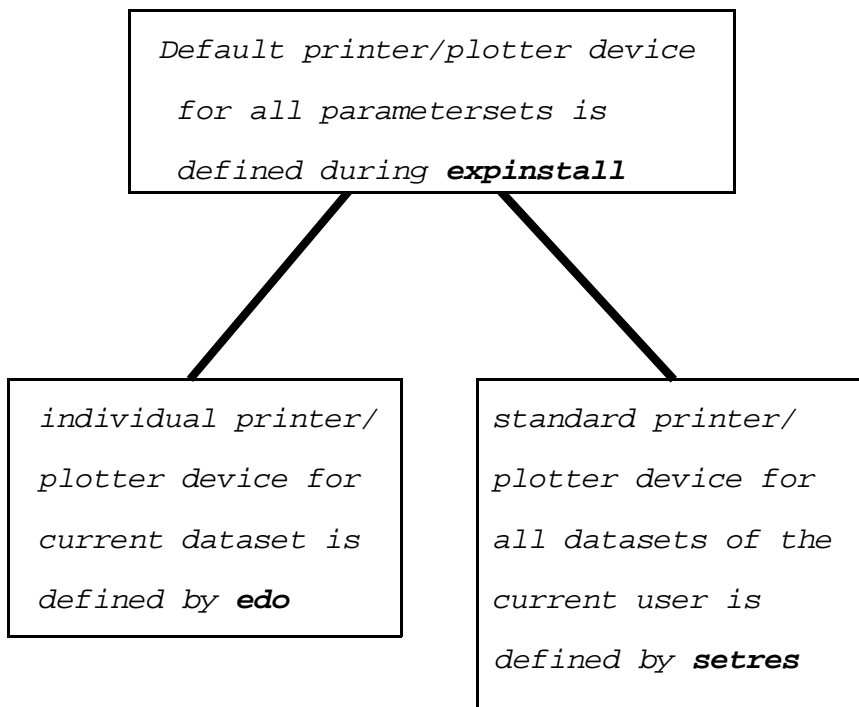
You will see:

- A list of all installed printers
- The entry '*Enhanced Metafile*'
- The entry '*Clipboard*'

Select one of these entries.

b) Type **edg** to setup the parameters

c) Type **plot** to plot the spectrum

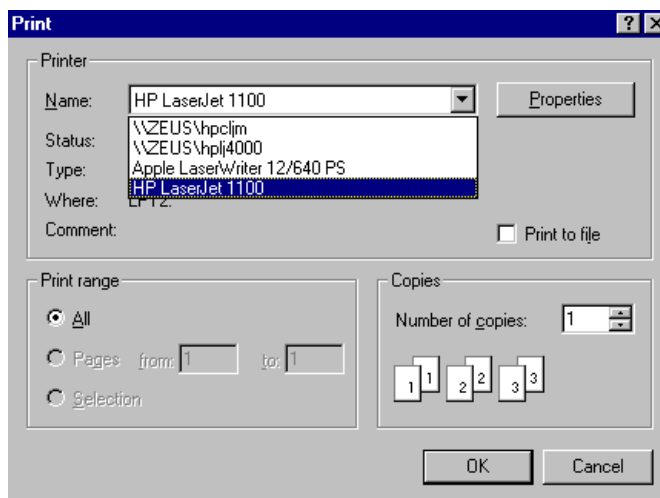


Note that the setting in **edo** only counts for the current dataset. The command

setres allows you to specify a general printer for all datasets of the current user. The printer setting in the **setres** window dominates the settings in **edo**, i. e. if you are fixed a printer device in **setres**, the plot command will be always send to this printer independently a different printer device in **edo**.

In XWIN-PLOT:

- a) Click **File** → **Print**
- b) select your desired printer in the pull down list to the right of **Name** field
- c) Click **OK**



17.1.3 Plotting from XWIN-NMR into Plot Files

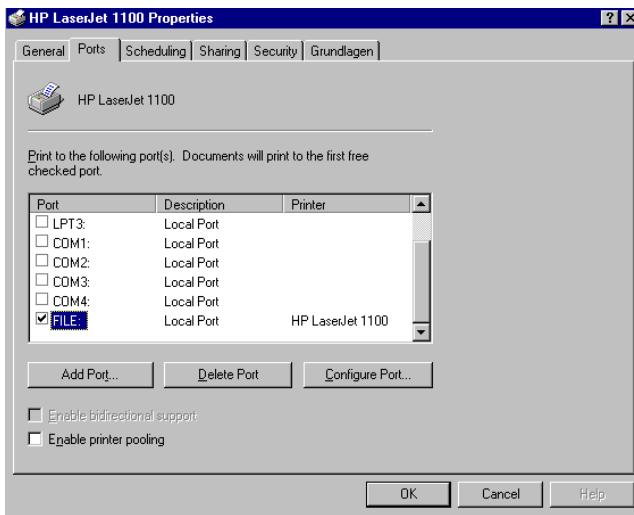
If no printer is connected to your computer, you can create Plot Files which can then be plotted from another computer, e.g. on a:

- Windows XP host with the command: `copy plot_file_name LPT1`
- UNIX host with the command: `cp plot_file_name /dev/plp`

You can create plot files in XWIN-NMR as follows:

1. Install the printer for which you want to create plot files, as described in chapter 6.1, but select **File** as the **port** or
2. Modify the port of an existing printer to **File**

- a) **Start** → **Settings** → **printers**
- b) Double-click on the printer for which you want to create plot files
- c) Click **Printer** → **Properties**
- d) Click **Ports** → select **File**



3. In XWIN-NMR:

- Enter: **edo** and select the printer which you installed in step 1
- Enter: **plot**

The name of a plot file consists of the creation date and time and the printer name, e.g. 980311121829-HP_LaserJet_4L.

Plot files are stored in the directory <XWINNMRHOME>\plotfiles. For a typical installation on the partition C: this is:

C:\Bruker\XWIN-NMR\plotfiles

You can store plot files in a different directory by setting the environment variable XWINNMRPLOTFILES in the following way:

1. Click **Start** → **Settings** → **Control Panel** → **Advanced**
2. Double-click the icon **Environment Variables**
3. A window 'Environment Variables' will appear:

- a) Click **New**
- 4. A window '*New User Variable*' will appear:
 - a) In the field **Variable Name**: enter **XWINNMRPLOTFILES**
 - b) In the field **Variable Value**: enter a directory of your choice, e.g.
C:\users\guest\plot
 - c) Click **OK** → **OK** → **OK**
- 5. Close the window '*Control Panel*' by clicking the **X** button

17.1.4 Plotting from XWIN-NMR into Enhanced Metafiles

XWIN-NMR supports the creation of Microsoft Windows Enhanced Metafiles. These can be read from any Microsoft program, e.g. Word, Powerpoint etc. You can create an Enhanced Metafile in the following way:

- a) Enter: **edo**
- b) Click the small arrow button to the right of the field CURPLOT
- c) Select Enhanced Metafile
- d) Enter: **plot**

The name of an Enhanced Metafile consists of the creation date and time and the extension .emf, e.g. 9803091621.emf. This file was created at 9 March 1998 at 16.21 PM.

Enhanced Metafiles are stored in the directory %XWINNMRHOME%\plotfiles. For a typical installation on partition C: this is C:\Bruker\XWIN-NMR\plot-files. If you want to store them in a different directory you must set the environment variable XWINNMRPLOTFILES as described in chapter 17.1.3.

17.1.5 Importing XWIN-NMR data into Microsoft programs

XWIN-NMR can plot the current dataset to the Windows XP Clipboard. From the Clipboard, data can easily be imported into Word, Powerpoint and other programs.

- 1. Write an XWIN-NMR dataset to the Clipboard:
 - a) Enter: **edo**
 - b) Click the small arrow button right of the field CURPLOT
 - c) Select: **Clipboard**
 - d) Click **SAVE**

e) Enter: **plot**

2. Read the dataset into a Microsoft program, e.g. in Word:

- Click **Edit** → **Paste**

Note that after step 1, the data can be viewed from the Clipboard by clicking the icon **Clip-board** on the screen

Instead of using the Clipboard, you can also store XWIN-NMR data into an Enhanced Metafile and import that into a Microsoft application as described in chapter 17.1.4

17.1.6 XWIN-PLOT

1. XWIN-PLOT uses the printer driver system of Windows XP for any printer output. This means that any printer for which a windows driver is correctly installed can be selected as print device. Note that the printer name in a layout file written by the Windows XP version is probably not known by the UNIX version of XWIN-PLOT because of the different printer handling. Apart from that, layout files can be freely interchanged between the two platforms.
2. XWIN-PLOT uses the Windows XP Clipboard. If you put one or more XWIN-PLOT objects to the Clipboard then these are stored in windows metafile format. Therefore any windows application which is able to read metafile data from the Clipboard can import XWIN-PLOT objects. XWIN-NMR 2.6 and newer can also import external graphics from the Clipboard.
3. Another way of exporting graphics is the menu option '*File/Export*' which allows you to save the complete layout in Windows Enhanced Metafile format (EMF). Most current graphical-oriented windows applications can import this format. This provides a convenient way of importing XWIN-PLOT graphics into programs like Word or Powerpoint.
4. Since XWIN-PLOT 2.6 you can directly send your current plot as Email. Just click **File** → **Send** and XWIN-PLOT will pop-up your default mail client and add the current plot as an EMF attachment.

Chapter 18

Windows XP commands

18.1 Online Help

Windows XP online help provides you with two kinds of help:

- help on specific topics
- help on what you see on your screen

18.1.1 Getting Help on specific topics

Click **Start** → **Help** (for a list of help topics)

- Click **Index** to get help on a predefined list of keywords
 - Enter the first letter(s) of a keyword
- Click **Find** to get help on all keywords contained in a data base

From the window which displays the help text you can go back to the main Help window by clicking **Help Topics**.

18.1.2 The question mark (?) in the upper right corner

Several windows, e.g. most windows which are opened from the Control Panel, have a question mark in the upper right corner. If you click it, the cursor will

change to an arrow with a question mark. Now you can click a button or field you want information about. The information will disappear when you click the desktop background.

18.1.3 Tips on Windows XP

This window appears every time you log in, unless you unselect

Show this screen at startup

If you want this window back: click **Start** → **Run** enter **welcome** click **OK**

Click in the right window to read some tips.

18.1.4 Windows XP tips and tricks on the Web

Innumerable tips and tricks on Windows XP can be found on various Web pages which are listed in chapter 21.7.

18.2 Command Prompt versus Graphical Interface

In a Windows environment, you normally work with a graphical interface, i.e. the **Start** button, Icons on the desktop, the Explorer etc. Nevertheless, Windows XP offers a Command Prompt, a shell, from which you can run various commands. The following table compares the Command Prompt with the graphical interface.

Function	Command Prompt	Graphical Interface
Files		
list files	dir	Explorer → Click Drive or Folder
delete a file	del (erase)	Right-click an icon in Explorer → Delete
rename a file	ren	Right-click an icon in Explorer → Rename
find text in files	find	Start → Search → For Files and Folders → Containing text
find a file		Start → Search → For Files and Folders → Search for Files or Folders

Function	Command Prompt	Graphical Interface
Directories		
make a dir.	mkdir (md)	File → New → Folder
remove a dir.	rmdir	Right-click icon in Explorer → Delete
change dir.	cd <dir>	Explorer
Utilities		
time and date	date, time	Start → Settings → Control Panel → Date/Time
backup	ntbackup	Start → Programs → Accessories → System Tools → Backup

18.3 Keyboard shortcuts

18.3.1 General Shortcuts

Function or mouse equivalent	Keyboard shortcut 1
Start	CTRL+ESC
Start → Documents	CTRL+ESC d
Start → Help	- CTRL+ESC h - F1 from desktop or explorer
Start → Run	- CTRL+ESC r - WIN+R
Start → Search	- CTRL+ESC c - F3 from desktop or explorer - WIN+F
Start → Shutdown	CTRL+ESC u
Taskbar → Task Manager	CTRL+SHIFT+ESC
Close the active window	ALT+F4 ¹
Close a hierarchy of windows	ALT+SHIFT+F4
Switch to other task	ALT+TAB
Minimize all windows on desktop	WIN+M
Restore all windows as seen before	WIN+SHIFT+M
Toggle normal/full-screen Command Prompt	ALT+ENTER
Copy entire screen to Clipboard	PRTSC (Print Screen)
Copy active window to Clipboard	ALT+PRTSC (Print Screen)

1. Be careful: If no window is active Windows XP will prompt for re-boot

18.3.2 Shortcuts for Windows Explorer

Function	Keyboard shortcut 1
Open new Explorer window	WIN+E
Rename file	F1
Open online help	F2
Open ' <i>Find</i> ' dialog	F3
Open ' <i>Folder</i> ' drop-down list	F4
Force refresh of windows contents	F5
Switch between left and right pane	F6
Go up one level in folder hierarchy	BACKSPACE
open context menu	- SFHIFT+F10 - right mouse click

18.4 Windows XP Command Prompt versus UNIX shell

Bruker BioSpin supports the NMR-SUITE for both UNIX and Windows XP. Here are some of the differences between these two operating systems which are of interest.

18.4.1 Directory specification

In a UNIX shell, pathnames are specified using the slash (/) character, whereas under Windows XP the backslash (\) character is used. Example:

UNIX shell: **cd /Bruker/XWIN-NMR**

Windows XP Command Prompt: **cd \Bruker\XWIN-NMR**

Under UNIX, command options are usually specified with a minus character (-) whereas in an Windows XP Command Prompt, the slash (/) character is used. For example, the command for listing files sorted by date:

UNIX shell: **ls -lrt**

Windows XP Command Prompt: **dir /od**

18.4.2 Windows XP commands versus UNIX commands

Under Windows XP, most commands can be executed via the Graphical Interface. You can, however, also open a Windows XP Command Prompt and run commands from there. Here is a list of UNIX shell commands and the corresponding Windows XP shell commands:

Function	UNIX shell	Windows XP Command Prompt
Files		
List files	ls	dir
copy a file	cp	copy
rename a file	mv	ren
delete a file	rm	del (erase)
print a file	lp	print
edit a file	vi, jot	notepad
display file contents	cat	type
sort a file	sort	sort
compare 2 files	diff	comp, fc
find text in file	grep	find
find a file	find	
Directories		
make a directory	mkdir	mkdir
remove a directory	rmdir	rmdir
copy a directory	cp -r	xcopy
change directory	cd <dir>	cd <dir>
show current directory	pwd	cd
Utilities		
time and date	date	date, time

Function	UNIX shell	Windows XP Command Prompt
manual pages	man	help
backup	tar	backup (floppy) or ntbackup (tape)

18.5 The UNIX GNU shell

For compatibility reasons, a UNIX shell is delivered on the NMR-SUITE CD and automatically installed during the installation of XWIN-NMR. When the installation is finished you can open a GNU shell by clicking:

Start → Programs → Bruker NMR Suite → GNU Shell

A GNU shell will open in which you can enter a restricted set of UNIX commands.

Chapter 19

Useful tools for Windows XP

This chapter contains a description of some tools we found useful. We realize that many other tools are available for various purposes and we are very interested in your experiences. Just send your comments to:

`nmr-software-support@bruker.de`

19.1 Update the operating system

There are two things that help you to be up-to-date with the operating system

- email notification about security fixes
- download and installation of hotfixes and service packs

19.1.1 Email notification about security fixes

Microsoft offers the possibility to subscribe for a newsletter that will inform you about security problems and their available fixes. Open Internet explorer and type in:

<http://register.microsoft.com/regsys/pic.asp>

You can subscribe there with your email address and after registration you can decide which kind of newsletter you want to get. It is recommended to subscribe at least for the:

Microsoft Security Notification Service

to get all information about security leaks and their fixes.

19.1.2 Update of the operating system

Open the Windows Explorer and click on **Tools** → **Windows Update**

- The Internet Explorer will open and show a page where you can choose to start the search for all necessary updates
- After the search is finished you have to choose which update of the available list you like to download
- Start the download and follow the instructions

19.2 Winzip: pack/unpack zip, tar, gz, uue files

The program Winzip allows you to pack or unpack archive files. The most common format is `.zip`, but Winzip also handles several other Windows and UNIX formats like `.tar`, `.gz` (created with `gzip`) and `.uue` (created with `uencode`). An Evaluation Version of WinZip is available at: www.winzip.com which can be used for viewing and extracting archives. For creating archives, you should order an official version. Once Winzip is installed, it is automatically started when you click a file with the extension `.zip`, `.tar`, `.gz`, `.uue` etc. You can also drag and drop the file's icon into the Winzip window. Then click **Extract** to extract one file from the archive or click **Checkout** to extract all files.

19.3 Defragment your disk

Windows XP has an own tool that allows you to defragment your disk. In the course of time your disk will become more and more fragmented. Although an NTFS partition (which is required for the NMR-SUITE), suffers much less from fragmentation than a FAT partition, it might be a good idea to defragment it from time to time.

Start → **Programs** → **Accessories** → **System Tools** → **Disk Defragmenter**

Chapter 20

Windows XP Tips and Tricks

20.1 Creating shortcut icons on the desktop

20.1.1 Creating shortcut icons to programs

For frequently used programs, it is convenient to create a shortcut icon on the desktop. For example, a shortcut to the editor **notepad** can be created as follows:

1. Right-click the **Start** button
2. Click **Open**
3. A window '*Start Menu*' will appear:
 - a) Double-click **All Programs**
 - b) Double-click **Accessories**
 - c) Press and hold the right mouse button on the **Notepad** icon
 - d) Drag the **Notepad** icon on the desktop, then release the right mouse button
 - e) Click **Create Shortcut(s) Here**

Alternatively, you can click **Start** → **Search** to find the executable file `Notepad.exe` and perform step c to e. (see also chapter 20.1.2)

20.1.2 Creating shortcut icons to documents/files:

For frequently used files, it is convenient to create a shortcut icon on the desktop. If Windows XP recognizes the extension of the file, the corresponding program to read the file will be started, e.g. Word for a .doc file. For a text file without extension, you can specify the program to be used. e.g. notepad, in the shortcut properties. As an example we will use the XWIN-NMR history file:

1. Find the directory <var>\prog\curdir\<user> in the Explorer
e.g. C:\Bruker\XWIN-NMR\prog\curdir\guest
2. Press and hold the right mouse button on the icon **history**
3. Drag the **history** icon on the desktop, then release the right mouse button
4. Click **Create Shortcut(s) Here**
→ an icon *Shortcut to history* will appear
5. Right-click the icon **Shortcut to history**
6. Click **Properties**
7. A window '*Shortcut to history properties*' will appear:
 - a) Click **Shortcut**
 - b) In the field **Target:** insert the program to be used before pathname, e.g.
notepad C:\Bruker\XWIN-NMR\prog\curdir\guest\history
 - c) Click **OK**

20.2 Convenient handling of XWIN-NMR under Windows XP

20.2.1 Reading data from the Explorer into XWIN-NMR

XWIN-NMR can read data from the Explorer, via the Clipboard. Perform the following steps:

- a) In the Explorer:
 - Find the dataset you want to display in XWIN-NMR
 - Right-click the data name folder
 - A popup window will appear: click **Copy**
- b) In XWIN-NMR:

- click **File** → **Paste**

You can also click a data expno or procno folder and read the corresponding dataset into XWIN-NMR.

20.2.2 Copy a text item into the XWIN-NMR command line

Any text item which can be copied to the Clipboard can be pasted to the XWIN-NMR command line. Of course this is only useful if this text item is an existing XWIN-NMR command. You can, for example, copy an XWIN-NMR command from the manual to the command line:

1. Click **Help** → **Complete Processing Manual**
2. The PDF viewer (if installed) will start up showing the XWIN-NMR processing manual:
 - a) Click **Tools** → **Select text**
 - b) Mark an XWIN-NMR command in the manual, e.g. **search**
 - c) Enter **Ctrl-C**
3. Move the cursor on the XWIN-NMR command line:
4. Click the middle mouse button.

This feature is especially useful for long command names or commands with many arguments. The text can come from various sources, e.g. online documents, the Command Prompt, text editors. You can, however, not copy file or program names directly from the Explorer to the XWIN-NMR command line.

Troubleshooting: if this feature does not work, please check if AutoCopy X Selection and Auto Paste to X Selection in Exceed are on (see chapter 10.3.1). Correct them if necessary and restart XWIN-NMR.

20.3 Various useful configurations

This paragraph describes several settings that we found useful. They have no influence on the NMR-SUITE performance and you are free to choose your own settings.

20.3.1 Configuring the Taskbar

1. Right-click the Taskbar ¹
2. Click **Properties**

3. A window '*Taskbar Properties*' will appear:
 - De-select the item **Always on top**, click **OK**

This will create more space on the desktop.

20.3.2 Hide known file extensions

See chapter 16.1.3

1. Open the Explorer
2. Click the menu **Tools** → **Folder Options**
3. In the '*Folder Options*' window:
 - a) Select **VIEW**
 - b) Unselect **Hide file extensions for known file types** (if it is selected)
 - c) Click **OK**

20.3.3 Show hidden files and folders

1. Open the Explorer
2. Click the menu **View** → **Options**
3. In the '*Folder Options*' window:
 - a) Select **VIEW**
 - b) Select **Show hidden files and Folders**
 - c) Click **OK**

20.3.4 Configuring the GNU shell

The GNU shell is delivered on the CD '*NMR-SUITE for Windows 2000 / Windows XP*' and is automatically installed together with the installation of XWIN-NMR. It provides a set of UNIX commands. By default, the resize and cut & paste functions are not active.

Making the GNU window resizable by default:

1. Click **Start** → **All Programs** → **Bruker TOPSPIN** → **GNU Shell**
2. A GNU shell window will appear:

1. The taskbar is usually, but not necessarily, at the bottom of the screen

- a) Click the symbol in the upper left corner of the window
- b) Click **Properties**
3. A window '*GNU shell properties*' will appear:
 - a) Click **Layout**
 - b) In the field Screen Buffer Size:
 - Set **Width** to 200
 - Set **Height** to 100
 - c) Click **OK**
4. A window '*Apply properties to shortcut*' appears:
 - a) Click **Modify shortcut which started this window**
 - b) Click **OK**

Enabling the cut & paste function:

1. Click **Start** → **All Programs** → **Bruker NMR Suite** → **GNU Shell**
2. A GNU shell window will appear:
 - a) Click the symbol in the upper left corner of the window
 - b) Click **Properties**
3. A window '*GNU shell properties*' will appear:
 - a) Click **Options**
 - b) Select **QuickEdit Mode**
4. A window '*Apply properties*' appears:
 - a) Click **Apply properties to current window only**
 - b) Click **OK**

The reason we do not recommend to enable the cut & paste function by default is that it would also count for the GNU shell started by XWIN-NMR. Accidentally using cut & paste in that window could cause XWIN-NMR to crash.

20.4 Connecting UNIX and Windows XP with Samba

Samba is a suite of programs which work together to allow clients to access UNIX file systems and printers via the SMB (Session Message Block) protocol.

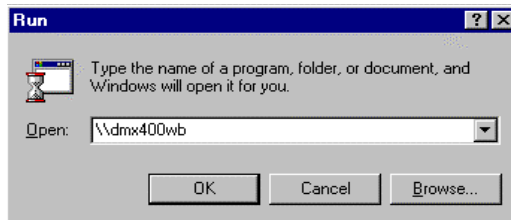
In practice, this means that you can 'share' disks and printers with UNIX systems. You can then access them from LanManager clients, Windows for Workgroups 3.11 clients, Windows95 clients, Windows NT clients, Windows XP clients and OS/2 clients. A 'share' is a term used to describe resources (directories, printers, etc.) that the server is making available for others on the network to use.

More information you may find in chapter 5.4.3, in the directory `/usr/samba/README` and `/usr/samba/docs` or if you have Internet access on <http://samba.org>

The license conditions are described in `/usr/samba/COPYING`.

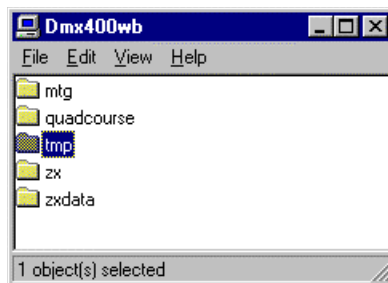
20.4.1 Accessing the network share provided by Samba

You can access shares from any Windows XP PC using the **Run...** feature available from the **Start** button.



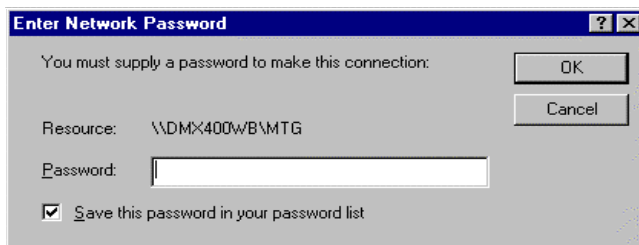
Type in two back-slashes followed by the (UNIX-)computer name (this operation is equivalent to running a '*find*' on a particular computer.

The corresponding response shows up in a Windows Explorer window:

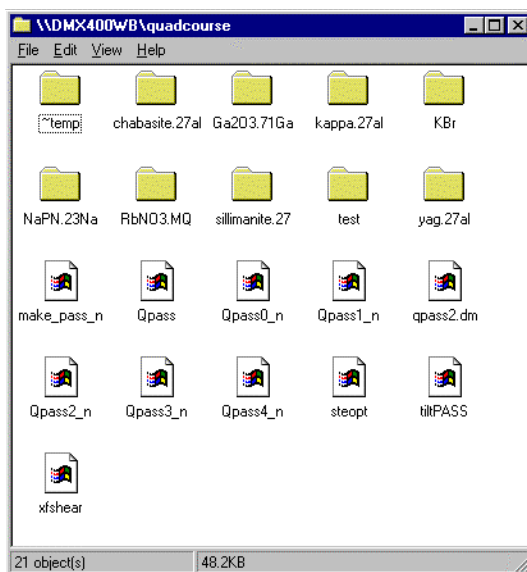


You can double-click on the share you want to see and it will come up with either a

password request for shares with managed access...



... or the list of contents (in yet another Explorer window):



If you cannot get access to a share that you see and you are confident that the password is correct please see chapters 20.4.3 and 20.4.4.

To copy files you can drag-and-drop them from a content display and deal with files and directories as if they were local (e.g. you can drag-and-drop acqu-files into a Wordpad-icon on you desktop. Technically the job of making a connection is completed here.

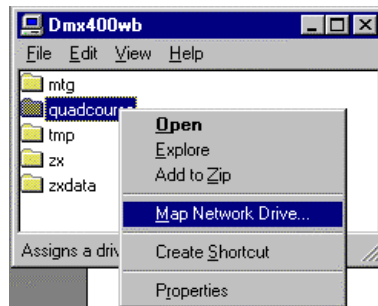
20.4.2 Mapping network shares into 'local' drives

For some applications (including XWIN-NMR) you will need, however, to map the

network share to a (virtual) disk drive. That is: You create a look-alike of a local drive like, say, U: that points to the share you assign to it.

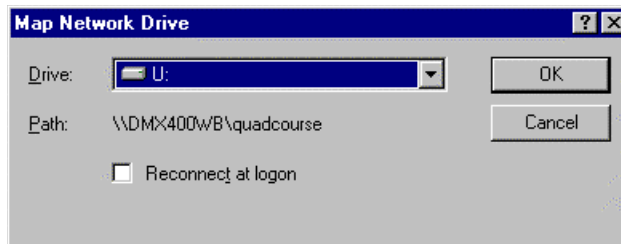
Doing this is very simple:

Step #1: click with the right mouse button on the share you want to map to a disk drive



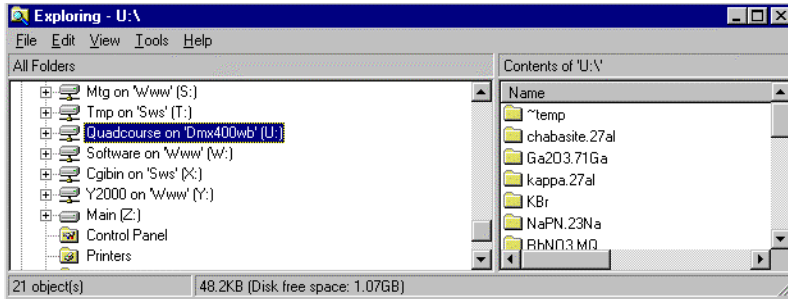
Select '**Map Network Drive**' (as shown).

Step #2: Select an appropriate drive letter (here: U:) and decide whether or not to click the '**reconnect at logon**' box. If you want a permanent connection that automatically is re-established any time the (client) PC is booting up click this box. If you don't check it this connection will only last until the next reboot.



Step #3: Press '**OK**'. As you press '**OK**' the system will connect this network share as a new drive called U: You can look up the new virtual disk in Windows

Explorer after a few seconds:



On the right-hand side the files shared out from UNIX are shown and you can go about copying, moving etc just like with native Windows files.

20.4.3 *Configuring Windows XP to handle UNIX-style password requests*

One of the most annoying problems with SAMBA is that older versions are not able to authenticate network connectors using encrypted passwords. In SAMBA 2.0.x the default setting is still plain password but you could change it to encrypted. This is the best way for the security of your network. If you want to use the plain-text password, it is possible on Windows XP side, to enable the authentication with clear-text passwords sent over the networking enabling the respective registry key (see the following chapters 20.4.5 and 20.4.4)

NOTE THAT THIS INTRODUCES A SIGNIFICANT SECURITY LEAK!

20.4.4 **Enable Plain Text Password**

1. Log in as administrator.
2. Click **Start** → **Control Panel**
3. Click **Administrative Tools** → **Local Security Policy**
4. Enable the tree **Local Policies** → **Security Options**
5. On the right side double click the entry '**Send unencrypted password to ...**'
6. Click on '**enabled**'
7. If your computer is part of a Windows NT / 2000 domain contact your domain administrator about this policy setting and its interaction with possible 'group policies'

20.4.5 There is one shortcut you can try with newer samba-versions

They deliver a file called *WinXP_PlainPassword.reg* in the *../samba/docs* directory. If you can locate this file in the Windows Explorer and double-click it, it will automatically make the additions to the registry file detailed hereafter. If you double-clicked the file and it worked you are done here. If not, you need to proceed as detailed in chapter 20.4.4 and manually make the necessary changes.

20.5 How to log on to Windows XP if you forget your password

20.5.1 Method 1: Log On as an Administrator and Reset the Password

If you can not log on to Windows by using a particular user account (including the Administrator or Computer Administrator accounts), but you can log on to another account with administrative privileges (including the Administrator or Computer Administrator accounts), follow these steps:

1. Log on to Windows by using the administrator account that has a password that you remember.

Note: You cannot log on as usual by using the Administrator or Computer Administrator account to a Windows XP Professional-based computer in a work-group. To log on as the Administrator or Computer Administrator, you must start Windows XP in Safe Mode.

2. Click **Start** → Click **Run**.
3. In the Open box, type the following command, and then click **OK**:
control userpasswords2
4. Click the user account that you forgot the password for → Click **Reset Password**.
5. Type a new password in both the New password and the confirm new password boxes → Click **OK**.

You should now be able to log on to Windows with the user account and the new password.

WARNING: If you reset the password for a user account in this manner in Windows XP Professional, the following types of information for that user will be no longer available:

- E-mail messages that are encrypted with the user's public key
- Internet passwords that are saved on, or remembered by, the computer
- Any files that the user has encrypted

20.5.2 Method 2: Use a Password Reset Disk

If you created a password reset disk for Windows XP, you are able to reset your password by using the password reset disk. For additional information about how to use a password reset disk, please check the articles in the Microsoft Knowledge Base:

- In order to create and use a Password Reset Disk for a computer that is not a domain member in Windows XP please read:

<http://support.microsoft.com/default.aspx?scid=kb;EN-US;305478>

- In order to create and use a Password Reset Disk for a computer in a domain in Windows XP please read:

<http://support.microsoft.com/default.aspx?scid=kb;EN-US;306214>

20.6 Error Message When You Use the Add Printer Wizard

When you create a printer (either a local printer or a remote network printer) by using the *Add Printer Wizard*, you may receive the following error message: "Operation could not be completed. The print spooler service is not running."

This error occurs because the Spooler service has not been started or has stopped working. To start the Spooler service, follow these steps:

1. Click **Start** → Click **Control Panel**.
2. Double-click **Administrative Tools** → Click **Services**.
3. Double-click the **Printer Spooler** service → Change the startup type to **Automatic**. This sets the Spooler service to start automatically when you restart the computer.
4. If you want to start the spooler service immediately, click the **Start** button under the **Service Status** field.

20.7 Internet Connection Firewall in Windows XP

Windows XP provides internet security in the form of a firewall (Internet Connection Firewall). This feature is designed for home and small business use and provides protection for computers directly connected to the Internet. This feature is available for local area network (LAN) or dial-up connections. It also prevents scanning of ports and resources (file and printer shares) from external sources.

20.7.1 Enable Internet Connection Firewall

a) **Use the Network Setup Wizard to enable the Internet Connection Firewall:**

1. Run the Network Setup Wizard.

Click **Start** → **Control Panel**, double-click **Network Connections**, and then click *Setup or change your home or small office network*.

2. The Firewall is enabled when you choose a configuration in the wizard that indicates that your computer is connected directly to the Internet.

b) **Configure the Internet Connection Firewall manually for a connection:**

1. Click **Start** → **Control Panel** → double-click **Network Connections**.

2. Right-click the connection on which you would like to enable the firewall → Click **Properties**.

3. On the **Advanced** tab, click the box to select the option to *Protect my computer or network*.

4. If you want to enable the use of some applications and services through the firewall, you need to enable them by clicking the **Settings** button. Then select the programs, protocols and services to be enabled for the firewall configuration.

20.7.2 Disable Internet Connection Firewall

1. Click **Start** → **Control Panel**, double-click **Network Connections**.

2. Right-click the connection on which you would like to disable the firewall → Click **Properties**.

3. On the **Advanced** tab, click the box to clear the option to *Protect my computer or network*.

Chapter 21

Appendix

21.1 Windows XP Important Information about your PC

1. *What is the Bruker BioSpin order number?*

HH _____

2. Customer details:

Name _____

Organization _____

Adr1 _____

Adr2 _____

Adr3 _____

3. Manufacturer and Type of the PC?

4. Manufacturer's system ID number of the PC?

5. Which service pack of Windows XP is installed: SP _____

(Shown at boot time on blue screen)

6. What type of graphics controller is installed?

7. Name of NMR SUPERUSER?

21.2 How do I remove a program?

One of the fundamental differences between UNIX and Windows XP is that application programs are much more closely interwoven with the Windows system files. Under UNIX, you have a fair chance uninstalling software by just removing the one directory that contained the executable(s).

Never, never, never delete directories under Windows to 'uninstall' software.

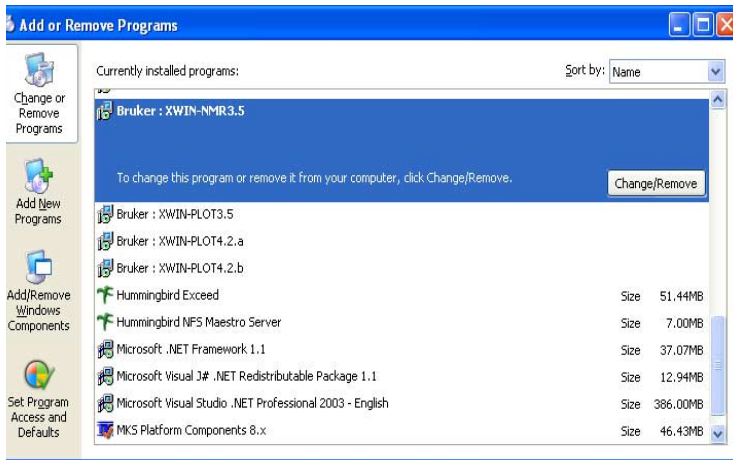
Many files that are uploaded during an installation go into other parts of the system or replace existing versions of files. Under Windows XP, an uninstall is more like a build-back and you need that to really clean things out.

As a preparation to make a build-back feasible all installation procedures leave behind log-files that tell the un-installer which files make up the product and where they have been placed. Furthermore, the uninstall procedure places a record into Windows' inventory of applications that you can simply start up and have it do the installation for you. That is the only way to uninstall applications under Windows you should ever consider. How does it work?

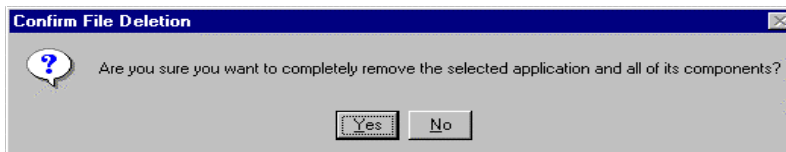
First call the 'Add/Remove Programs' icon from the Control Panel:



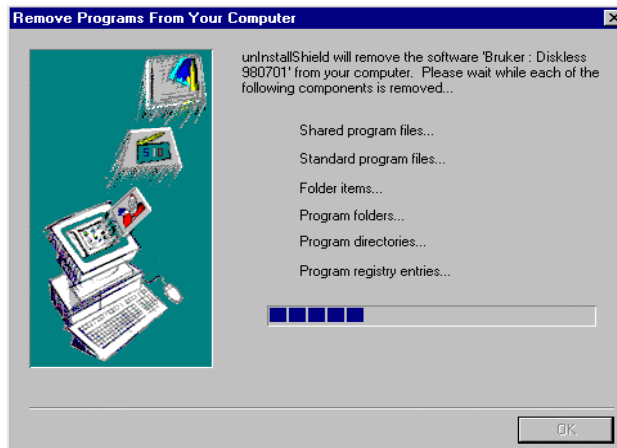
Then make your pick from the list of applications and press the button labeled 'Change/Remove':



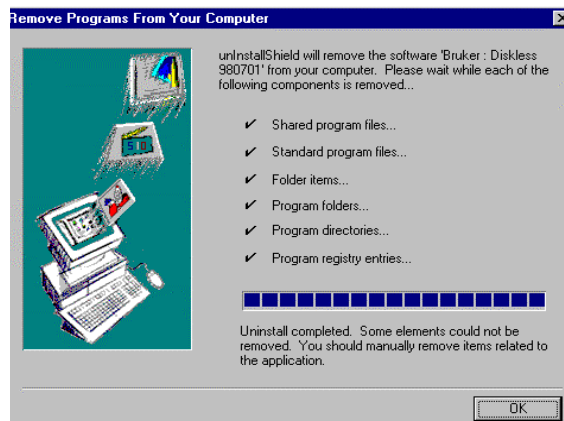
In most cases the first thing you will see is the are-you-sure-you-want-to-proceed?-prompt. Those vary in shape and text but most likely every product will have one:



Once confirmed the actual un-installation process starts and you will see progress messages:



Important: Sometimes you are prompted whether or not you want to delete certain components. These are mostly shared libraries that sit in system directories and may or may not be used by other components. Please leave them in the system, do NOT delete them except you are absolutely positive that they belong to the current installation only. In many cases you can tell from the filename or its location in a sub-directory of the applications home spot that this is a safe thing. If in doubt, leave them on - with 10-15 Gigabytes you can afford to lose a few hundred Kilo-byte here. After all you normally don't un-install three dozen applications. Eventually all the different aspects of removing a piece of software are automatically covered by the un-installer and the OK button comes up to take your confirmation:



Please note that all the items with check-marks have been worked on by the un-installer. If you would have just wiped out the directory with the application, then the rest would still litter the system disk and command and control units.

Click OK to finish the job.

Note: Sometimes you find that after an un-install parts of the directory structure and some files are still in the original place where the application had resided. That is done on purpose. The idea is that you, for example, do not want to wipe out your precious license file just because you put on a new version of flexlm. Or loose datasets in \u\data because the XWIN-NMR version gets updated.

21.3 Configure Input Focus 'Move With Mouse'

The 'input focus' is the window or spot on your desktop that receives characters you type on your keyboard. Under Windows the window whose title bar is coloured (default: blue) is the window that has the input focus. You can shift the input focus to another window by clicking on it once. That will make it's title bar change from gray (no focus) to color (has focus).

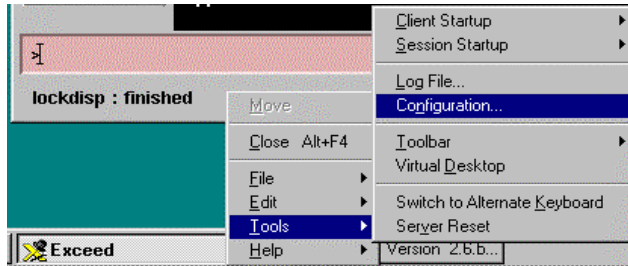
Many people, however, prefer a different setting for their NMR related activities: They would rather like to see the input focus automatically shift to any window as the mouse gets moved over it. This is the default used for X-Windows in a UNIX-based environment. There are pros and cons to both concepts. This chapter explains how to alter the input focus policy we can have for our NMR applications.

Note: Please understand that the automatic focus shift per mouse-over is not a Windows-feature. It is made possible by the Exceed-emulation we use for our XWIN-NMR program and will apply only to windows that are part of XWIN-NMR.

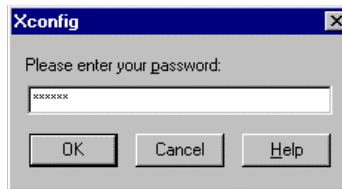
Bruker BioSpin does not recommends to change the input focus policy

To alter the settings you need to run the Exceed-server. It is automatically started with XWIN-NMR and will stay running even as you terminate XWIN-NMR. Locate

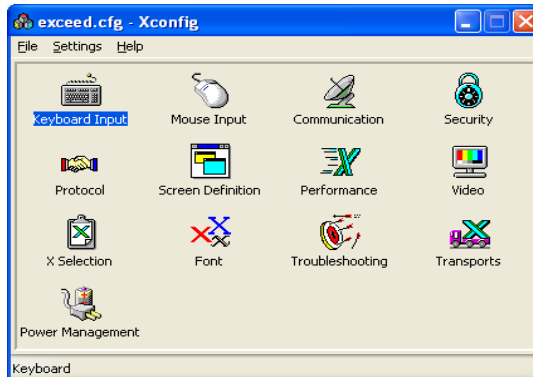
the Exceed icon on your taskbar and right-click on it to get the following menu:



Select Tools/Configuration. You will be prompted for the Exceed-password you put on during installation of Exceed:

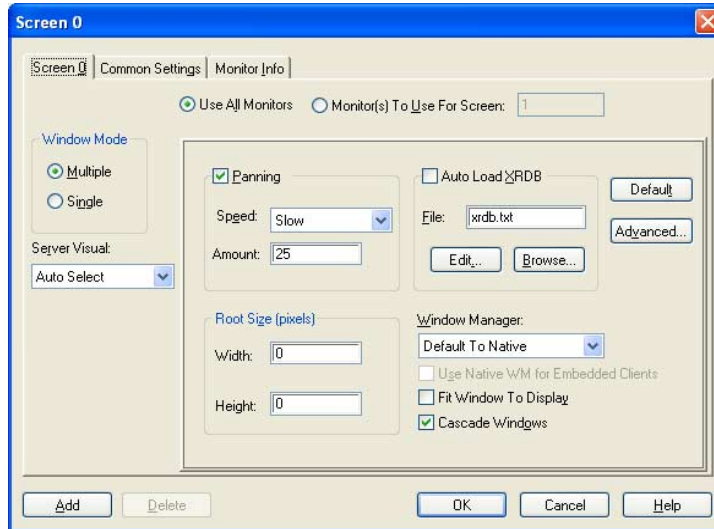


Press OK when the password is entered. This will bring up all configuration settings for Exceed:

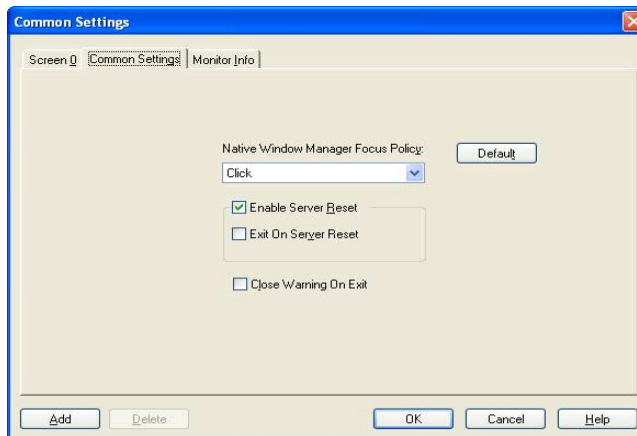


Please select 'screen definition' to bring up the relevant dialogue-box for setting the

input focus. In this box select the 'common settings' tab:



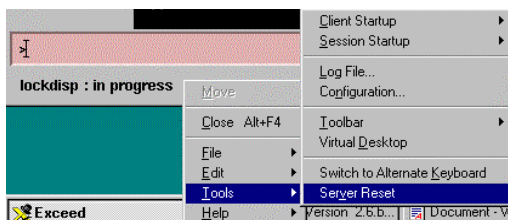
Most likely the default setting is 'click' which means you have to click on a window to make the input focus go to that window:



To change the input focus policy, please click on the little arrow to pull down the menu. Then press 'OK' to apply the new setting. If you want to get back to the windows default at some point please come back to this screen and set it to 'click'.

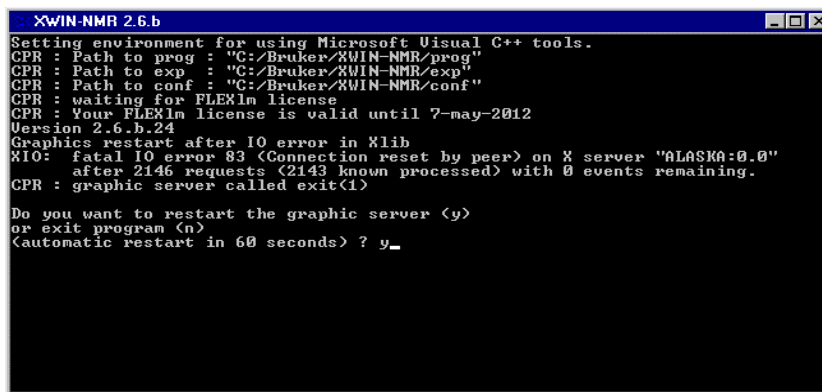
Now you have to force the already-running eXceed-server into adopting our new

setting. You can achieve that by resetting the server:



As before, locate the server icon on the taskbar and right-click for the menu. This time choose 'Server Reset' as shown above.

If X-related windows are open (for example your XWIN-NMR, a lock display or the like) you will receive a warning that the Exceed-server will shut them all down as it resets. That's OK. Just confirm the warning. If you had XWIN-NMR running you will see the start-up text window expose the messages for a graphics restart:



Type 'y' and then press the enter-key on your keyboard. This will bring XWIN-NMR back up and the change to focus policy that you made above will already be in effect.

21.4 Some notes for the helium handling

In the XWIN-NMR installation path (normally C:\Bruker\XWIN-NMR) in the directory ... \prog\logfiles are two files named heliumlog and heliumlog.err. The heliumlog saves every night at 3.00 am the actual helium level in a new line. The heliumlog.err documents every error during detecting the helium level.

21.4.1 Automatic notification for helium refill

1. Open a Command Prompt and enter:

- `cd /d c:\Bruker\XWIN-NMR`
- `notepad heliumlimit`

type in the number (without '%') of the helium level should activate the notification, e. g. **25**

click **file** → **save as ..** and save it as **<XWINNMRHOME>\heliumlimit**

Of course, you can also install the heliumlimit file from the Explorer. We have chosen the Command Prompt because the Explorer might add the (perhaps hidden) extension `.txt` to the file `heliumlevel` which makes it unusable (see chapter 12.2.3).

2. Now you could create a command script `<XWINNMRHOME>\heliumwarn.cmd` that will be executed if the actual helium level is the same or below the entry (in %) in the file `<XWINNMRHOME>\heliumlimit`

E. g. it is possible to create a message window on the screen of the spectrometer PC and/or every other PC in your network (e. g. the PC of the responsible person for helium refill). You could do this in the following way:

3. Open a Command Prompt and enter:

- `cd /d c:\Bruker\XWIN-NMR`
- `notepad heliumwarn.cmd`

type in the following text:

```
@echo off
rem -----
rem heliumwarn.cmd: example MS cmd script to send a warning
rem                  argument1=LEVEL
rem                  argument2=LIMIT
rem -----
rem  user defined variables:
rem  INSTRUMENT: is the name of the spectrometer
rem  ADDRESS    : the address where the message is sent to.
rem                  type 'net help send' for details
rem -----
```

```

set INSTRUMENT='Avance-300'
set ADDRESS1=%COMPUTERNAME%
set ADDRESS2=%NMR-SUPERUSER-PC%
set ADDRESS3=%HELIUM-REFILLER-PC%
rem -----
rem  catch command line arguments:
rem -----
set MYSELF=%0
set LEVEL=%1
set LIMIT=%2
rem -----
rem  get the name of the spectrometer host:
rem -----
set HOST=%COMPUTERNAME%
rem -----
rem  prepare the email message:
rem -----
set MSG=Attention: At the magnet of the %INSTRUMENT% spec-
trometer is the heliumlevel of %LEVEL%% equal or lower than
the helium level limit of %LIMIT%%: please order liquid he-
lium and refill the helium tank. --- This message has been
sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and
%ADDRESS3%
rem -----
rem  send the message:
rem -----
net send %ADDRESS1% %MSG%
net send %ADDRESS2% %MSG%
net send %ADDRESS3% %MSG%

```

You have to write in your individual parameters

- replace Avance-300 with the name of your spectrometer
- replace NMR-SUPERUSER-PC with the name of the PC of the NMR-Superuser

- replace HELIUM-REFILLER-PC with the name of the PC of the responsible person for helium refill
- Attention - the text sequence:

set MSG=Attention: At the magnet of the %INSTRUMENT% spectrometer is the heliumlevel of %LEVEL%% equal or lower than the helium level limit of %LIMIT%%: please order liquid helium and refill the helium tank. --- This message has been sent by %MYSELF% on %HOST% to %ADDRESS1%, %ADDRESS2% and %ADDRESS3%

had to be written in one line!

Click **file** → **save as..** and save it as <XWINNMRHOME>\heliumwarn.cmd

Now the defined PC's will get an error message if the actual helium level is the same or below the entry (in %) in the file <XWINNMRHOME>\heliumlimit

The notifications were sends only once but it will be activated again if the helium level is against higher than the limit.

Note that this script is only an example, if you would like to add more PC's in the notification list you had to add the respective addresses, if you like to have less addresses you have to delete the respective entries.

21.4.2 Helium measurement under Windows XP Service Pack 1

On Windows XP SP1 the nightly heliumlog does not work. The reason is a bug in Microsoft Service Pack 1 which lets the task scheduler execute only those jobs which run under the account of the user who is currently logged on. See the article in the Microsoft knowledge base:

<http://support.microsoft.com/default.aspx?scid=kb;en-us;812400>

If there is always the same user logged on all the time, then workaround no. 1 can be applied. Otherwise use the 2nd workaround.

- Possibility 1: The helium log runs under the local system account. Change this to the user who is always logged on:
 - Click on **Start** → **Control Panel** → **Task Scheduler**.
 - Doubleclick on the task AT1(2,...) which runs at 3:00 AM. Specify the user name besides 'Run as:' and set the password accordingly (the user must have a password!)
 - Click **OK**.

- Possibility 2: Disable the HID-Service (Human Interface Device Access) and restart the computer.

Note: Remove this modified task before installing a new XWIN-NMR version.

21.5 Upper/Lower case letters

The Windows XP file system NTFS intentionally does not differentiate between upper and lower case letters. Therefore working on a PC, please observe the following:

1. if you want to work with your SGI spectra on a PC avoid to create datasets with the same name differentiated only by being written in upper or lower case letters.
2. do not ignore the upper and lower case letters of NMR-SUITE commands. If for instance you type **rpar PROT*** Xwin-nmr will display the rpar-list of all parameter sets beginning with 'PROT'. The command **rpar Prot*** will show no parameter list, although the MS-Explorer displays the parameter set 'PROTON' in the wrong way 'Proton'

21.6 Books on Windows XP

If you want to learn more about Windows XP, you can choose from various books on the subject both for users and system administrators. Several of them are delivered with a CDROM containing training or Windows XP applications (like the Windows XP resource kit). For prices, descriptions and ordering information we refer to the following Web site:

- <http://store.yahoo.com/softpro>
- <http://shop.microsoft.com>

21.7 Web pages on Windows XP

Most of the web pages below were recommended by the eLetter (www.executive.com/eletter).

- <http://www.microsoft.com/windowsXP/default.asp>
- <http://support.microsoft.com>

Chapter 22

Bruker BioSpin addresses

Germany

Bruker BioSpin GmbH
Silberstreifen
D-76287 Rheinstetten
Tel: (++49) (721) 51 61 0
Fax: (++49) (721) 51 71 01

Bruker BioSpin Software Department
Silberstreifen
D-76287 Rheinstetten
Tel: (++49) (721) 5161 455
Fax: (++49) (721) 5161 943

<http://www.bruker-biospin.de>

ftp server: <ftp.bruker.de>

Email: nmr@bruker-biospin.de (sales)
mbu@bruker.de (service)
applik@bruker.de (application)
nmr-software-support@bruker-biospin.de (software)
license@bruker.de (licenses)

USA

Bruker BioSpin Corporation
15 Fortune Drive
Manning Road
Billerica, MA. 01821-3991

Tel: (++1)(978) 667 9580 5195 (center)
 (++1)(978) 667 9580 5444 (application)
Fax: (++1)(978) 667 6168 (center)
 (++1)(978) 667 2955 (application)

<http://www.bruker-biospin.com>

ftp server: <ftp.bruker.com>

Email: applab@bruker.com
 center@bruker.com
 software@bruker.com

Switzerland

Bruker BioSpin AG
Industriestraße 26
CH-8117 Fällanden

Tel: (++41)(1) 8 25 91 11
Fax: (++41)(1) 8 25 96 96

web server: www.bruker.ch

E-Mail: epweb@bruker.ch
 all_ap@bruker.ch

France

Bruker BioSpin S.A.
34, rue de l'industrie
F-67166 Wissembourg/Cedex

Tel: (++33)(3) 88 73 68 00
Fax: (++33)(3) 88 73 68 79

web server: www.bruker.fr

E-Mail: support-rmn@bruker.fr (customer support)

England

Bruker BioSpin LTD.

Banner lane

Coventry CV4 9GH

Tel: (++44)(2476) 855200

Fax: (++44)(2476) 465317

web server: www.bruker.co.uk

Email: service@bruker.co.uk

apps@bruker.co.uk

Our webpage

<http://www.bruker-biospin.de/NMR/about/offices/index.html>

- provides contact addresses of our facilities and offices worldwide

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